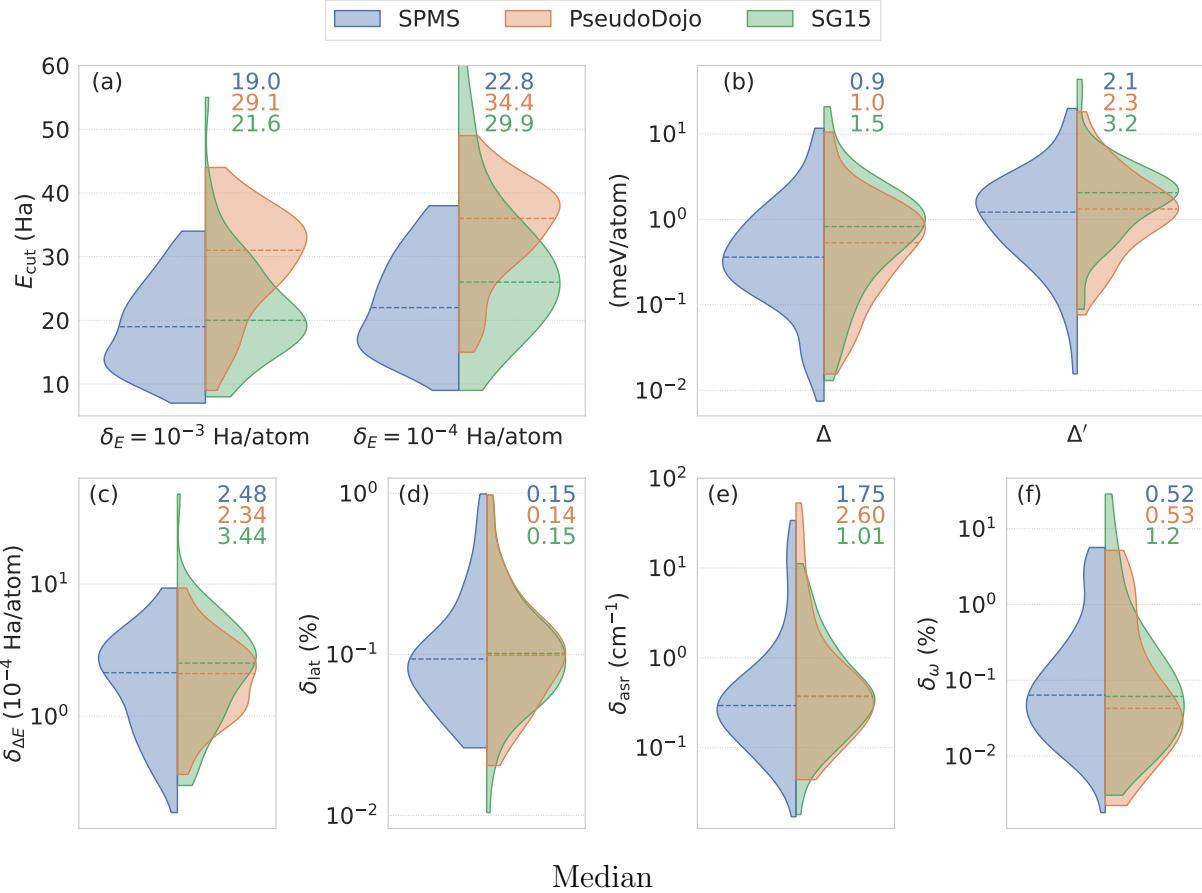


# SPMS pseudopotentials v1.0

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Mostafa Faghah Shojaei, John E. Pask, Andrew J. Medford, and Phanish Suryanarayana.

“Soft and transferable pseudopotentials from multi-objective optimization.”  
arXiv preprint arXiv:2209.09806 (2022). (<https://doi.org/10.1016/j.cpc.2022.108594>)  
Acknowledgment: U.S. Department of Energy (DOE), Office of Science (SC): DE-SC0019410



Median

|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 19.0                 | 22.0                 | 2.13                | 0.36     | 1.21      | 0.06                  | 0.08 | 0.10 | 0.27                  | 0.31 | 0.07              | 0.06 |
| PseudoDojo | 31.0                 | 36.0                 | 2.10                | 0.53     | 1.32      | 0.08                  | 0.09 | 0.10 | 0.40                  | 0.33 | 0.04              | 0.04 |
| SG15       | 20.0                 | 26.0                 | 2.52                | 0.83     | 2.05      | 0.09                  | 0.09 | 0.09 | 0.32                  | 0.40 | 0.07              | 0.05 |

Mean

|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 19.0                 | 22.8                 | 2.48                | 0.94     | 2.13      | 0.18                  | 0.15 | 0.11 | 1.99                  | 1.50 | 0.65              | 0.39 |
| PseudoDojo | 29.1                 | 34.4                 | 2.34                | 0.98     | 2.26      | 0.18                  | 0.14 | 0.11 | 2.92                  | 2.27 | 0.69              | 0.37 |
| SG15       | 21.6                 | 29.9                 | 3.44                | 1.50     | 3.20      | 0.19                  | 0.15 | 0.10 | 1.02                  | 1.00 | 1.46              | 0.93 |

$\delta_E$ : Convergence error of the total energy in Ha/atom

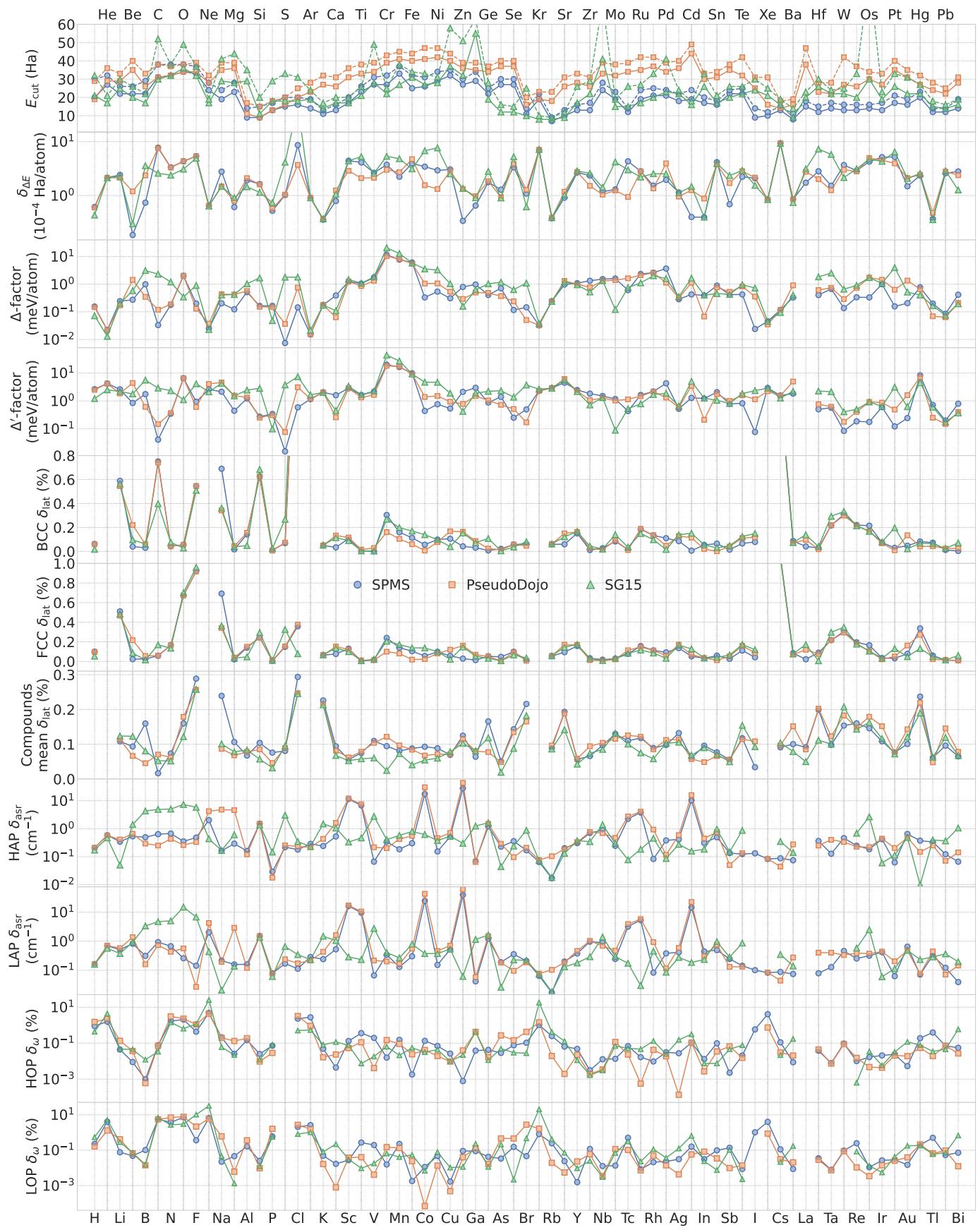
$\delta_{\Delta E}$ : The accuracy metric in  $10^{-4}$  Ha/atom used for SPMS optimization.

$\Delta$  and  $\Delta'$ : The  $\Delta$ -factor and  $\Delta'$ -factor in meV/atom.

$\delta_{\text{lat}}$ : Mean of absolute value of percentage lattice constant errors for BCC, FCC, and compound (COMP) structures used to test the GBRV table

$\delta_{\text{asr}}$ : Mean of absolute value of acoustic sum rule errors in  $\text{cm}^{-1}$  for the highest and lowest acoustic phonon frequencies (HAP and LAP) at  $\Gamma$ -point obtained for the  $\Delta$ -factor lattice structures

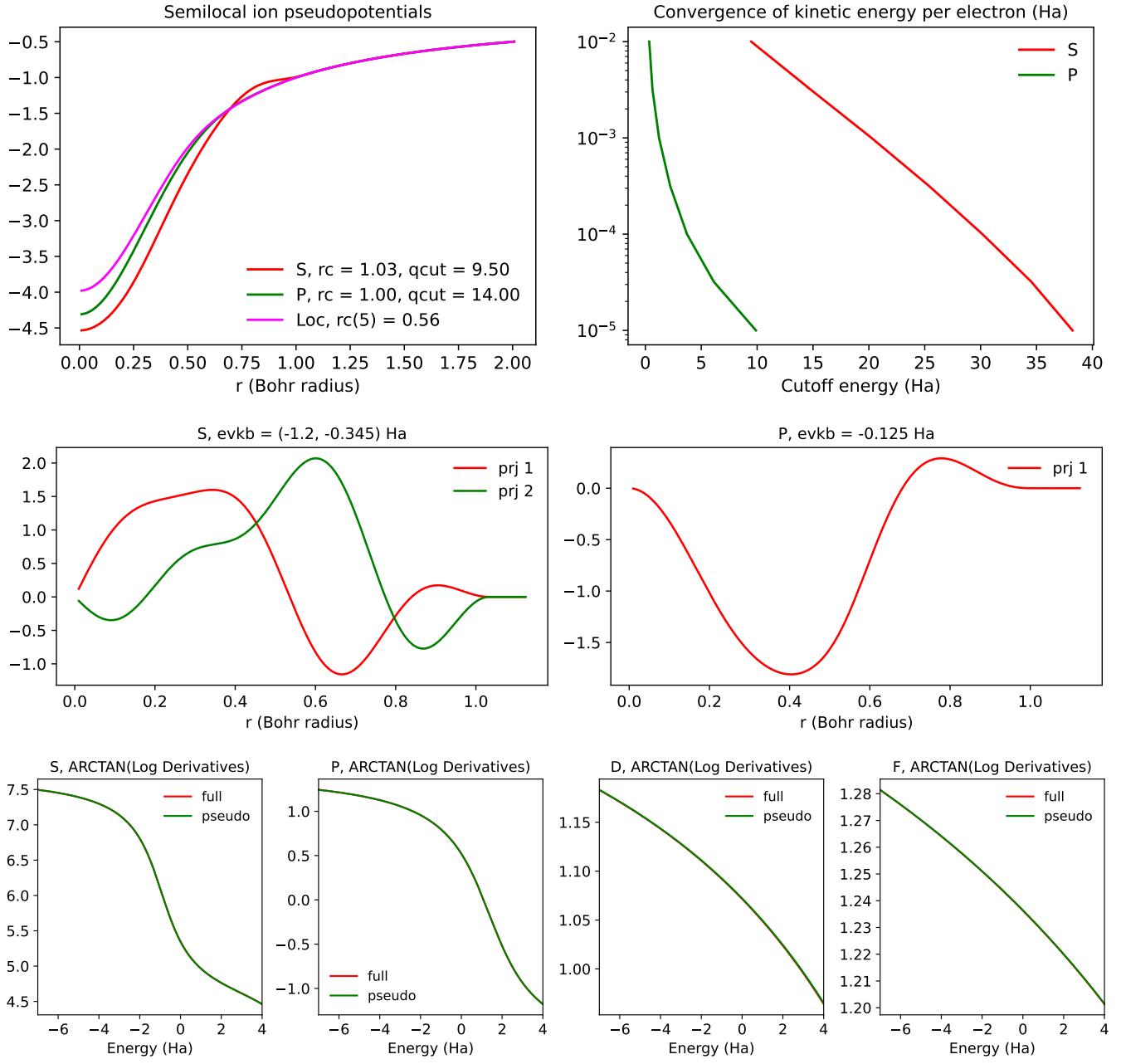
$\delta_{\omega}$ : Mean of absolute value of percentage phonon frequency errors for the highest and lowest optical phonon frequencies (HOP and LOP) obtained after imposing the acoustic sum rule at  $\Gamma$ -point for the  $\Delta$ -factor lattice structures and  $E_{\text{cut}}$  corresponding to  $\delta_E = 10^{-4}$  Ha/atom



# SPMS

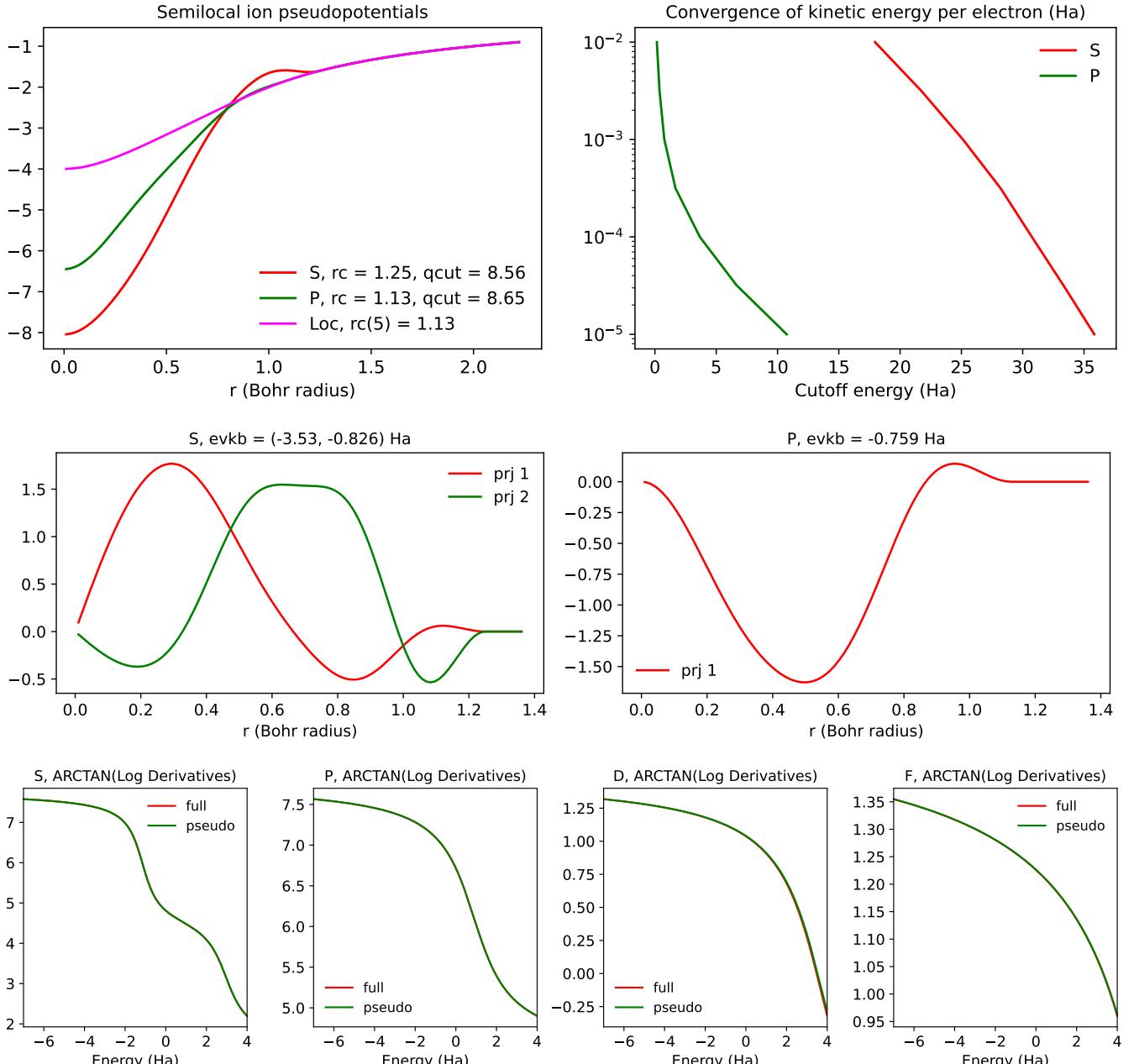
|    | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |       | $\delta_{\omega}$ |      |
|----|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|-------|-------------------|------|
|    | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP   | LOP               | HOP  |
| H  | 20                   | 30                   | 0.61                | 0.16     | 2.62      | 0.06                  | 0.10 | -    | 0.16                  | 0.21  | 0.23              | 0.90 |
| He | 27                   | 32                   | 2.13                | 0.02     | 4.18      | -                     | -    | -    | 0.69                  | 0.59  | 4.10              | 1.58 |
| Li | 22                   | 26                   | 2.42                | 0.24     | 2.59      | 0.59                  | 0.51 | 0.11 | 0.52                  | 0.34  | 0.08              | 0.04 |
| Be | 22                   | 26                   | 0.19                | 0.27     | 0.84      | 0.04                  | 0.02 | 0.09 | 0.82                  | 0.54  | 0.05              | 0.01 |
| B  | 22                   | 29                   | 0.74                | 0.99     | 1.75      | 0.03                  | 0.03 | 0.16 | 0.31                  | 0.50  | 0.10              | 0.00 |
| C  | 31                   | 38                   | 7.71                | 0.03     | 0.04      | 0.75                  | 0.06 | 0.02 | 0.93                  | 0.64  | 5.58              | 0.08 |
| N  | 32                   | 38                   | 3.34                | 0.18     | 0.35      | 0.04                  | 0.16 | 0.07 | 0.67                  | 0.67  | 3.74              | 1.70 |
| O  | 34                   | 38                   | 4.30                | 2.02     | 6.51      | 0.06                  | 0.67 | 0.16 | 0.26                  | 0.35  | 7.21              | 2.05 |
| F  | 33                   | 37                   | 5.36                | 0.20     | 0.93      | 0.55                  | 0.92 | 0.29 | 0.14                  | 0.48  | 0.36              | 0.44 |
| Ne | 24                   | 28                   | 0.65                | 0.03     | 2.56      | -                     | -    | -    | 2.03                  | 2.03  | 6.54              | 4.78 |
| Na | 19                   | 24                   | 2.77                | 0.20     | 2.13      | 0.69                  | 0.69 | 0.24 | 0.22                  | 0.16  | 0.02              | 0.21 |
| Mg | 23                   | 28                   | 0.61                | 0.12     | 0.44      | 0.02                  | 0.02 | 0.11 | 0.16                  | 0.29  | 0.05              | 0.03 |
| Al | 9                    | 14                   | 1.92                | 0.52     | 1.21      | 0.14                  | 0.14 | 0.07 | 0.16                  | 0.16  | 0.17              | 0.15 |
| Si | 9                    | 15                   | 1.63                | 0.16     | 0.27      | 0.63                  | 0.24 | 0.10 | 1.51                  | 1.51  | 0.03              | 0.03 |
| P  | 13                   | 17                   | 0.52                | 0.17     | 0.34      | 0.01                  | 0.00 | 0.08 | 0.08                  | 0.03  | 0.60              | 0.07 |
| S  | 15                   | 20                   | 1.02                | 0.01     | 0.02      | 0.07                  | 0.15 | 0.08 | 0.17                  | 0.22  | -                 | -    |
| Cl | 16                   | 20                   | 8.62                | 0.14     | 0.59      | 2.31                  | 0.36 | 0.29 | 0.11                  | 0.18  | 2.08              | 2.32 |
| Ar | 14                   | 19                   | 0.90                | 0.02     | 1.16      | -                     | -    | -    | 0.29                  | 0.29  | 2.62              | 2.74 |
| K  | 11                   | 13                   | 0.36                | 0.18     | 2.03      | 0.05                  | 0.06 | 0.23 | 0.24                  | 0.24  | 0.05              | 0.05 |
| Ca | 13                   | 16                   | 0.79                | 0.39     | 1.60      | 0.03                  | 0.08 | 0.09 | 0.53                  | 0.53  | 0.02              | 0.00 |
| Sc | 17                   | 20                   | 4.43                | 1.25     | 2.84      | 0.11                  | 0.13 | 0.06 | 16.41                 | 11.61 | 0.03              | 0.13 |
| Ti | 23                   | 26                   | 4.12                | 1.05     | 1.63      | 0.00                  | 0.00 | 0.07 | 9.63                  | 6.80  | 0.27              | 0.36 |
| V  | 27                   | 31                   | 2.64                | 1.75     | 2.15      | 0.00                  | 0.02 | 0.11 | 0.07                  | 0.07  | 0.20              | 0.20 |
| Cr | 27                   | 32                   | 3.74                | 11.65    | 19.80     | 0.30                  | 0.24 | 0.09 | 0.34                  | 0.34  | 0.02              | 0.02 |
| Mn | 33                   | 37                   | 2.23                | 7.75     | 16.33     | 0.16                  | 0.14 | 0.08 | 0.13                  | 0.18  | 0.23              | 0.15 |
| Fe | 25                   | 32                   | 3.93                | 6.12     | 9.75      | 0.11                  | 0.10 | 0.09 | 0.30                  | 0.30  | 0.00              | 0.00 |
| Co | 26                   | 31                   | 3.43                | 0.33     | 0.44      | 0.06                  | 0.06 | 0.09 | 24.73                 | 17.49 | 0.01              | 0.13 |
| Ni | 29                   | 34                   | 2.93                | 0.54     | 0.76      | 0.10                  | 0.10 | 0.09 | 0.15                  | 0.15  | 0.05              | 0.07 |
| Cu | 32                   | 35                   | 3.05                | 0.31     | 0.54      | 0.11                  | 0.06 | 0.07 | 0.52                  | 0.52  | 0.00              | 0.03 |
| Zn | 27                   | 30                   | 0.34                | 0.80     | 2.11      | 0.04                  | 0.03 | 0.12 | 39.60                 | 28.00 | 0.09              | 0.00 |
| Ga | 29                   | 34                   | 0.65                | 0.97     | 2.94      | 0.03                  | 0.01 | 0.06 | 0.04                  | 0.07  | 0.09              | 0.04 |
| Ge | 22                   | 25                   | 1.77                | 0.41     | 0.87      | 0.01                  | 0.05 | 0.17 | 1.21                  | 1.21  | 0.04              | 0.04 |
| As | 27                   | 30                   | 1.28                | 0.71     | 1.39      | 0.02                  | 0.05 | 0.05 | 0.19                  | 0.23  | 0.03              | 0.03 |
| Se | 27                   | 30                   | 3.35                | 0.12     | 0.25      | 0.06                  | 0.10 | 0.14 | 0.36                  | 0.36  | 0.15              | 0.08 |
| Br | 11                   | 14                   | 1.09                | 0.15     | 0.49      | 0.06                  | 0.01 | 0.22 | 0.21                  | 0.17  | 0.05              | 0.11 |
| Kr | 19                   | 22                   | 7.04                | 0.03     | 2.27      | -                     | -    | -    | 0.06                  | 0.06  | 0.82              | 1.02 |
| Rb | 7                    | 9                    | 0.38                | 0.24     | 2.90      | 0.06                  | 0.05 | 0.09 | 0.02                  | 0.02  | 0.25              | 0.25 |
| Sr | 10                   | 13                   | 0.92                | 0.97     | 4.48      | 0.06                  | 0.09 | 0.19 | 0.20                  | 0.20  | 0.02              | 0.06 |
| Y  | 13                   | 16                   | 2.67                | 1.09     | 2.46      | 0.15                  | 0.16 | 0.06 | 0.38                  | 0.31  | 0.00              | 0.05 |
| Zr | 13                   | 17                   | 2.35                | 1.33     | 1.82      | 0.01                  | 0.03 | 0.07 | 0.97                  | 0.70  | 0.12              | 0.00 |
| Nb | 24                   | 28                   | 1.18                | 1.53     | 1.50      | 0.03                  | 0.02 | 0.10 | 0.88                  | 0.88  | 0.01              | 0.01 |
| Mo | 19                   | 23                   | 1.30                | 1.60     | 1.17      | 0.08                  | 0.03 | 0.13 | 0.25                  | 0.25  | 0.01              | 0.01 |
| Tc | 12                   | 14                   | 4.32                | 0.61     | 0.43      | 0.02                  | 0.08 | 0.11 | 3.21                  | 2.27  | 0.50              | 0.07 |
| Ru | 19                   | 24                   | 2.81                | 2.35     | 1.63      | 0.19                  | 0.16 | 0.12 | 5.38                  | 3.80  | 0.01              | 0.02 |
| Rh | 21                   | 25                   | 1.53                | 2.61     | 2.17      | 0.13                  | 0.11 | 0.09 | 0.08                  | 0.08  | 0.02              | 0.01 |
| Pd | 21                   | 24                   | 1.95                | 3.70     | 4.27      | 0.11                  | 0.09 | 0.10 | 0.38                  | 0.38  | 0.02              | 0.03 |
| Ag | 18                   | 22                   | 1.14                | 0.29     | 0.52      | 0.09                  | 0.14 | 0.13 | 0.42                  | 0.42  | 0.03              | 0.03 |
| Cd | 19                   | 24                   | 0.40                | 0.43     | 1.28      | 0.01                  | 0.05 | 0.06 | 14.72                 | 10.41 | 0.16              | 0.11 |
| In | 17                   | 20                   | 0.40                | 0.39     | 1.22      | 0.05                  | 0.03 | 0.10 | 0.44                  | 0.31  | 0.03              | 0.01 |
| Sn | 16                   | 18                   | 4.16                | 0.89     | 2.05      | 0.06                  | 0.06 | 0.08 | 0.50                  | 0.50  | 0.10              | 0.10 |
| Sb | 22                   | 24                   | 0.69                | 0.42     | 0.78      | 0.01                  | 0.03 | 0.06 | 0.25                  | 0.13  | 0.14              | 0.00 |
| Te | 22                   | 25                   | 2.23                | 0.43     | 0.82      | 0.07                  | 0.11 | 0.12 | 0.14                  | 0.12  | 0.01              | 0.02 |
| I  | 9                    | 14                   | 2.09                | 0.02     | 0.08      | 0.08                  | 0.04 | 0.03 | 0.10                  | 0.13  | 1.03              | 0.58 |
| Xe | 10                   | 12                   | 0.84                | 0.05     | 2.90      | -                     | -    | -    | 0.08                  | 0.08  | 4.01              | 4.10 |
| Cs | 13                   | 15                   | 9.33                | 0.12     | 1.56      | 1.34                  | 1.07 | 0.09 | 0.09                  | 0.09  | 0.11              | 0.11 |
| Ba | 8                    | 11                   | 0.85                | 0.33     | 1.82      | 0.09                  | 0.08 | 0.10 | 0.07                  | 0.07  | 0.01              | 0.01 |
| La | 15                   | 18                   | 1.73                | -        | -         | 0.04                  | 0.02 | 0.09 | -                     | -     | -                 | -    |
| Hf | 12                   | 15                   | 2.82                | 0.40     | 0.50      | 0.03                  | 0.09 | 0.20 | 0.08                  | 0.36  | 0.03              | 0.04 |
| Ta | 14                   | 17                   | 1.52                | 0.67     | 0.57      | 0.22                  | 0.22 | 0.10 | 0.13                  | 0.13  | 0.01              | 0.01 |
| W  | 13                   | 16                   | 3.68                | 0.14     | 0.08      | 0.31                  | 0.30 | 0.15 | 0.46                  | 0.46  | 0.09              | 0.09 |
| Re | 13                   | 16                   | 2.89                | 0.34     | 0.19      | 0.22                  | 0.19 | 0.16 | 0.25                  | 0.25  | 0.25              | 0.01 |
| Os | 14                   | 16                   | 4.26                | 0.33     | 0.18      | 0.21                  | 0.17 | 0.15 | 0.32                  | 0.18  | 0.01              | 0.02 |
| Ir | 13                   | 17                   | 5.15                | 1.00     | 0.60      | 0.07                  | 0.03 | 0.11 | 0.42                  | 0.42  | 0.03              | 0.02 |
| Pt | 17                   | 21                   | 5.19                | 0.16     | 0.12      | 0.03                  | 0.03 | 0.08 | 0.06                  | 0.06  | 0.03              | 0.02 |
| Au | 16                   | 19                   | 1.48                | 0.21     | 0.24      | 0.05                  | 0.08 | 0.10 | 0.65                  | 0.65  | 0.01              | 0.01 |
| Hg | 20                   | 23                   | 2.35                | 0.77     | 8.24      | 0.08                  | 0.34 | 0.24 | 0.07                  | 0.37  | 0.20              | 0.19 |
| Tl | 12                   | 14                   | 0.37                | 0.20     | 0.71      | 0.07                  | 0.06 | 0.06 | 0.33                  | 0.34  | 0.50              | 0.39 |
| Pb | 12                   | 14                   | 2.59                | 0.08     | 0.20      | 0.01                  | 0.01 | 0.10 | 0.12                  | 0.12  | 0.05              | 0.07 |
| Bi | 14                   | 19                   | 2.79                | 0.42     | 0.79      | 0.00                  | 0.01 | 0.07 | 0.04                  | 0.07  | 0.07              | 0.06 |

# Hydrogen (H)



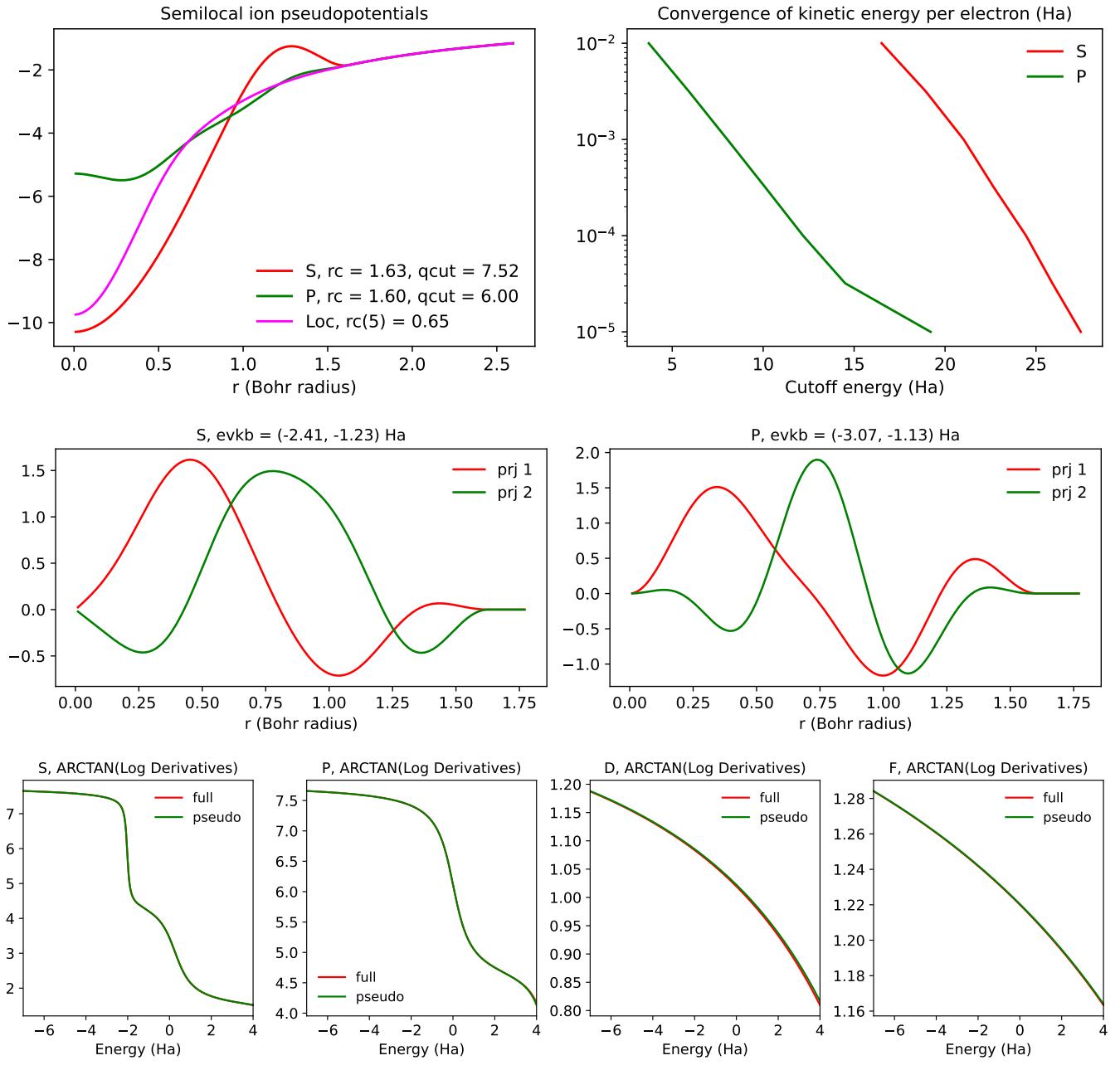
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 20                   | 30                   | 0.61                | 0.16     | 2.62      | 0.06                  | 0.10 | -    | 0.16                  | 0.21 | 0.23              | 0.90 |
| PseudoDojo | 19                   | 29                   | 0.60                | 0.15     | 2.49      | 0.06                  | 0.10 | -    | 0.16                  | 0.21 | 0.16              | 1.53 |
| SG15       | 21                   | 32                   | 0.43                | 0.07     | 1.21      | 0.02                  | 0.05 | -    | 0.16                  | 0.17 | 0.55              | 0.43 |

# Helium (He)



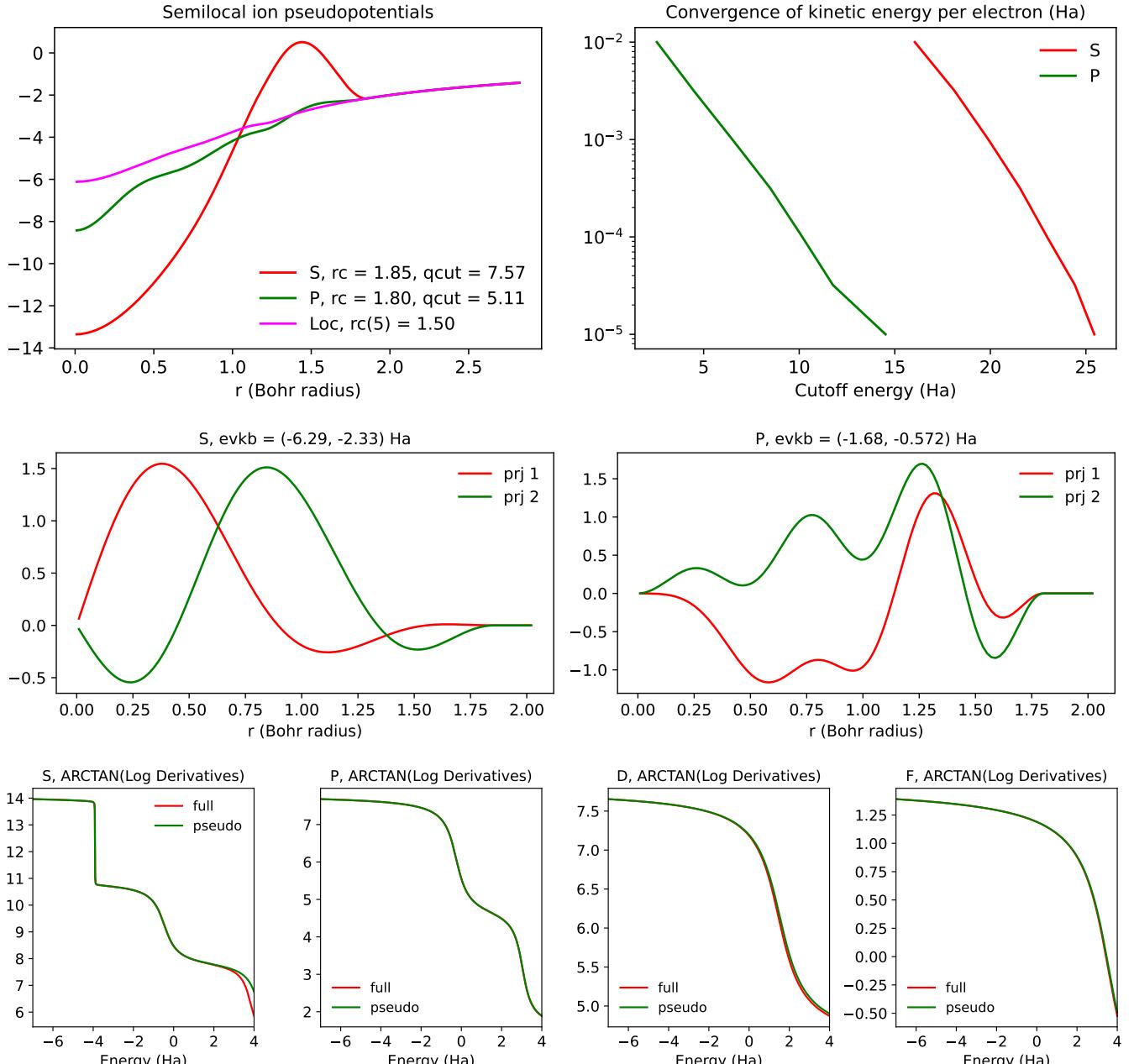
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |     |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|-----|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 27                   | 32                   | 2.13                | 0.02     | 4.18      | -                     | -   | -    | 0.69                  | 0.59 | 4.10              | 1.58 |
| PseudoDojo | 29                   | 36                   | 2.13                | 0.02     | 4.16      | -                     | -   | -    | 0.71                  | 0.57 | 1.30              | 2.22 |
| SG15       | 17                   | 21                   | 2.13                | 0.01     | 2.49      | -                     | -   | -    | 0.57                  | 0.47 | 5.14              | 4.42 |

# Lithium (Li)



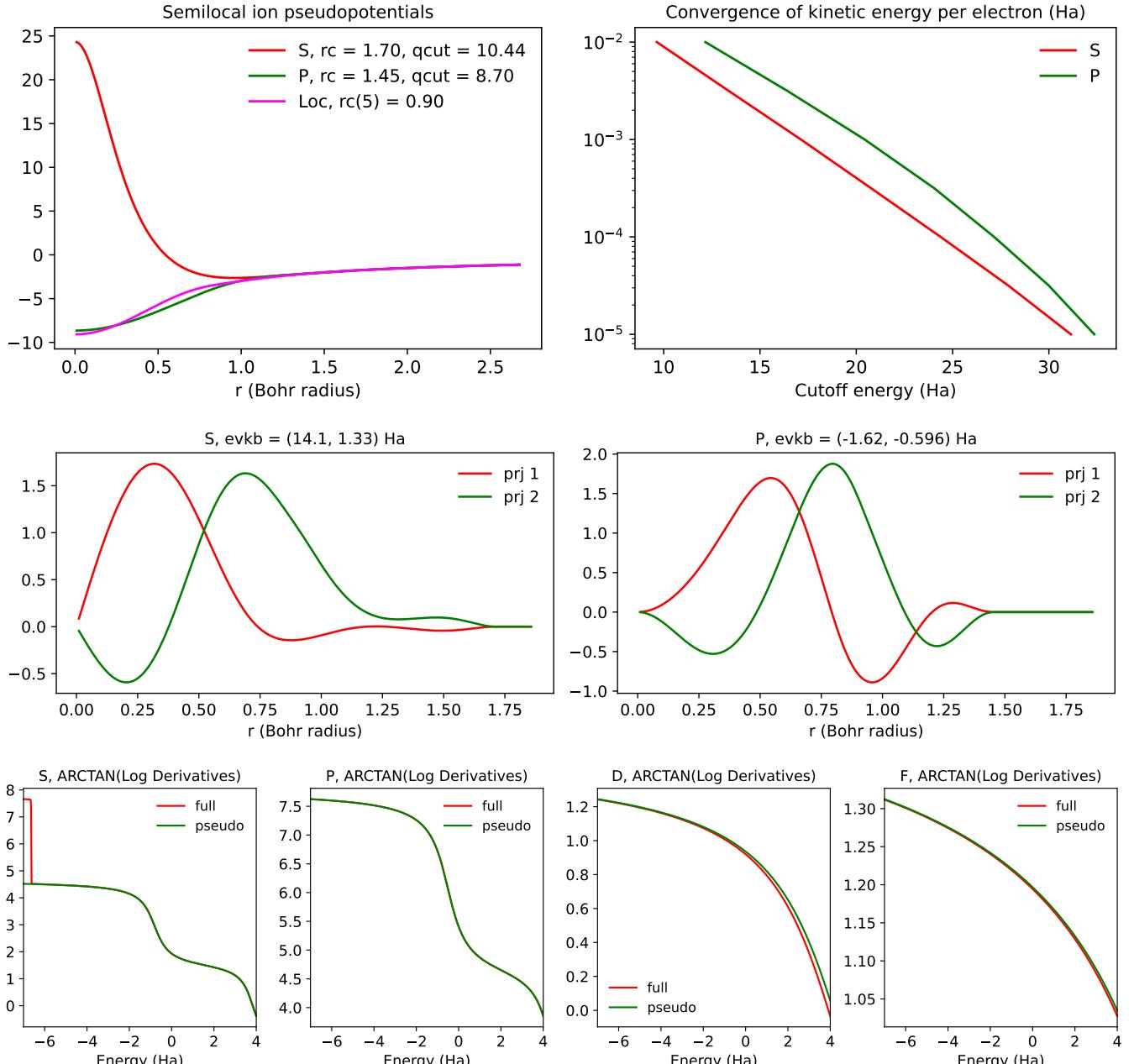
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 22                   | 26                   | 2.42                | 0.24     | 2.59      | 0.59                  | 0.51 | 0.11 | 0.52                  | 0.34 | 0.08              | 0.04 |
| PseudoDojo | 29                   | 33                   | 2.14                | 0.17     | 1.85      | 0.54                  | 0.47 | 0.11 | 0.58                  | 0.41 | 0.41              | 0.13 |
| SG15       | 25                   | 30                   | 2.27                | 0.20     | 2.17      | 0.56                  | 0.48 | 0.12 | 0.38                  | 0.05 | 0.29              | 0.05 |

# Beryllium (Be)



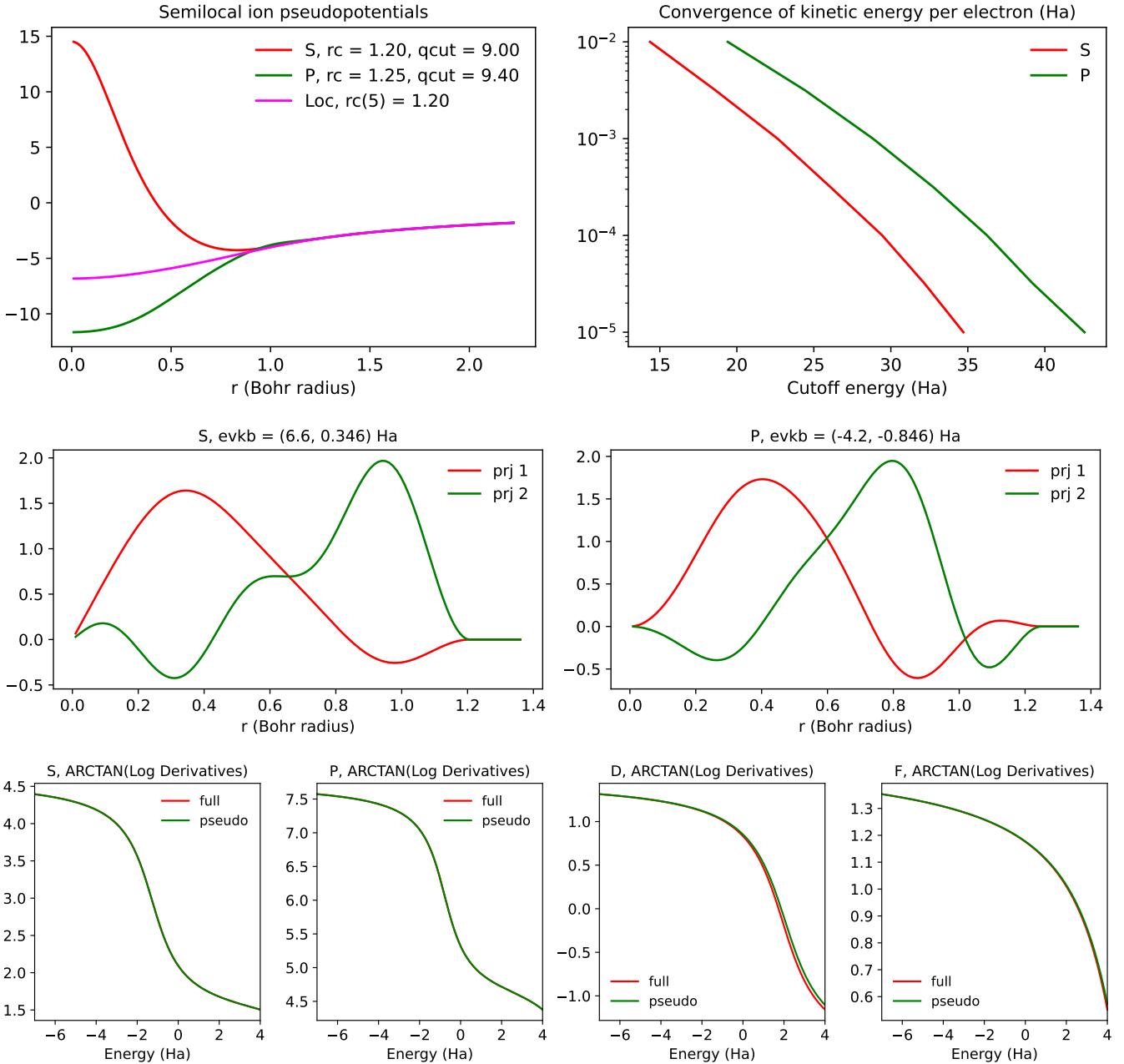
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 22                   | 26                   | 0.19                | 0.27     | 0.84      | 0.04                  | 0.02 | 0.09 | 0.82                  | 0.54 | 0.05              | 0.01 |
| PseudoDojo | 35                   | 40                   | 1.20                | 1.44     | 4.38      | 0.22                  | 0.22 | 0.07 | 1.38                  | 0.66 | 0.07              | 0.04 |
| SG15       | 20                   | 26                   | 0.30                | 0.58     | 1.78      | 0.10                  | 0.08 | 0.12 | 0.93                  | 1.42 | 0.07              | 0.04 |

# Boron (B)



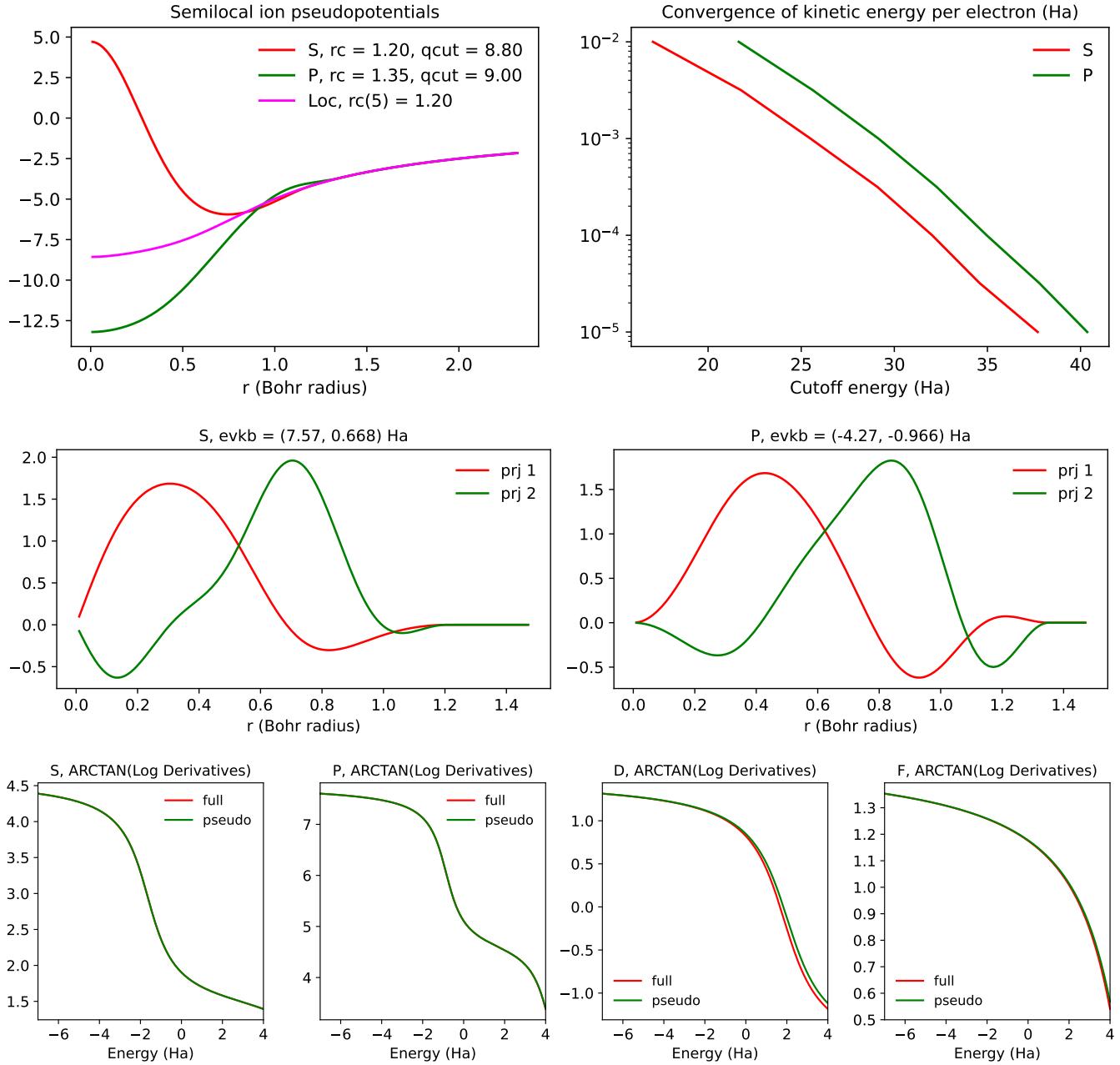
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 22                   | 29                   | 0.74                | 0.99     | 1.75      | 0.03                  | 0.03 | 0.16 | 0.31                  | 0.50 | 0.10              | 0.00 |
| PseudoDojo | 26                   | 33                   | 2.36                | 0.35     | 0.61      | 0.06                  | 0.06 | 0.05 | 0.16                  | 0.29 | 0.01              | 0.00 |
| SG15       | 17                   | 22                   | 3.58                | 3.13     | 5.55      | 0.06                  | 0.01 | 0.08 | 3.36                  | 4.32 | 0.02              | 0.01 |

# Carbon (C)



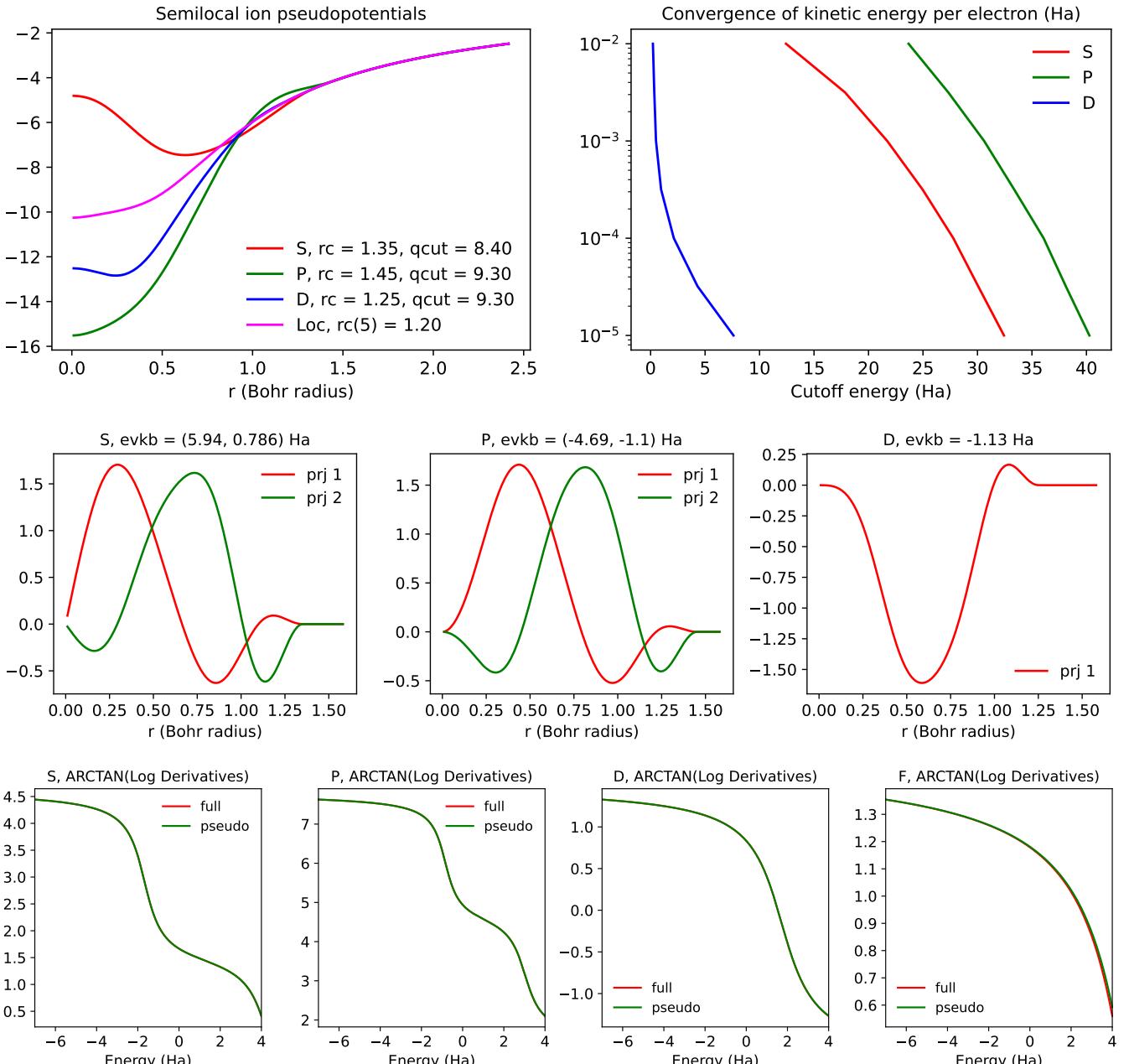
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 31                   | 38                   | 7.71                | 0.03     | 0.04      | 0.75                  | 0.06 | 0.02 | 0.93                  | 0.64 | 5.58              | 0.08 |
| PseudoDojo | 31                   | 38                   | 7.59                | 0.12     | 0.15      | 0.74                  | 0.06 | 0.07 | 0.74                  | 0.25 | 5.56              | 0.07 |
| SG15       | 30                   | 52                   | 2.59                | 2.31     | 2.88      | 0.40                  | 0.17 | 0.05 | 4.74                  | 4.91 | 6.84              | 0.03 |

# Nitrogen (N)



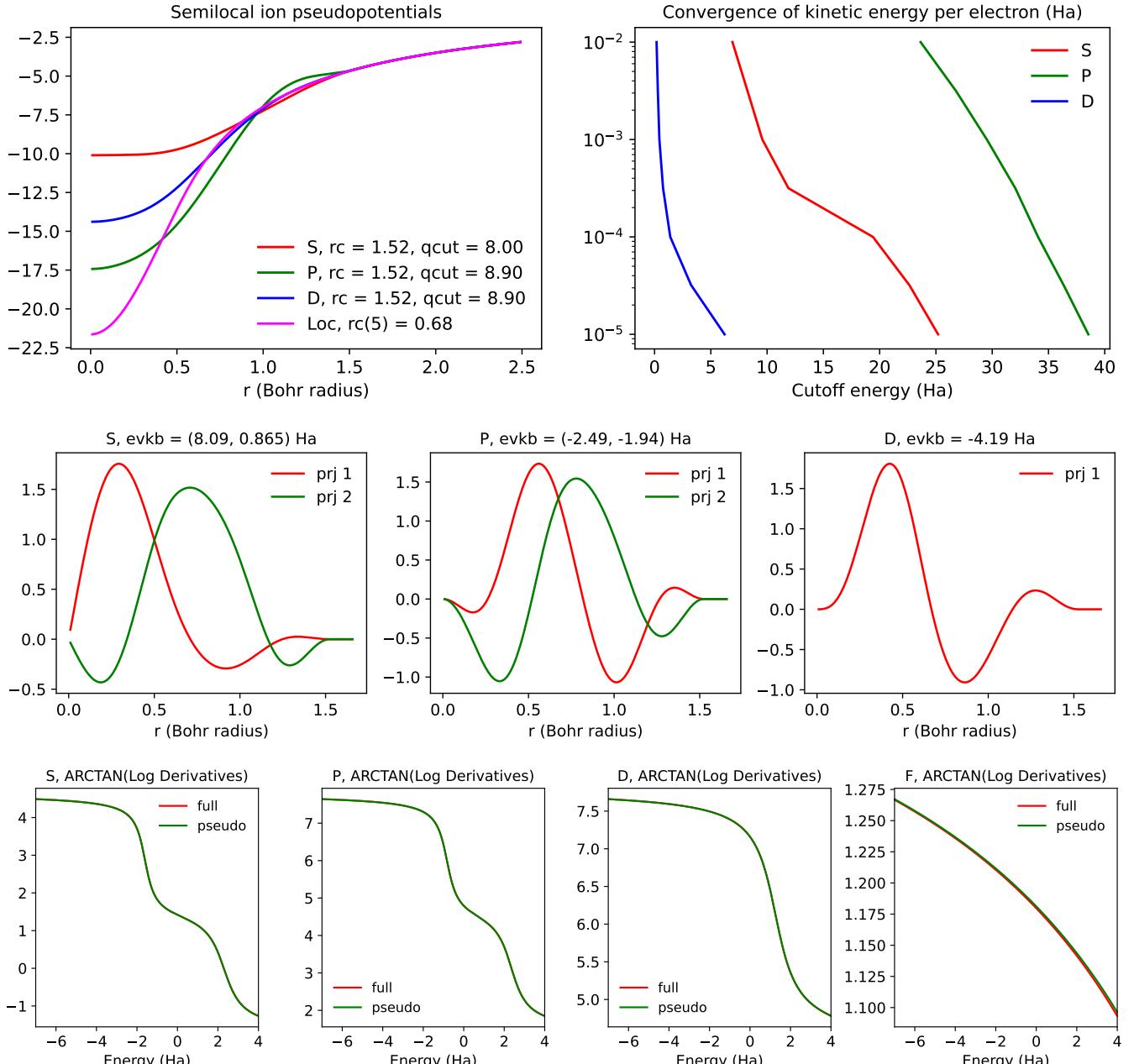
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 32                   | 38                   | 3.34                | 0.18     | 0.35      | 0.04                  | 0.16 | 0.07 | 0.67                  | 0.67 | 3.74              | 1.70 |
| PseudoDojo | 32                   | 37                   | 3.31                | 0.19     | 0.37      | 0.04                  | 0.16 | 0.06 | 0.43                  | 0.43 | 7.05              | 3.08 |
| SG15       | 32                   | 38                   | 2.39                | 1.20     | 2.32      | 0.08                  | 0.14 | 0.05 | 5.05                  | 5.05 | 2.71              | 1.44 |

# Oxygen (O)



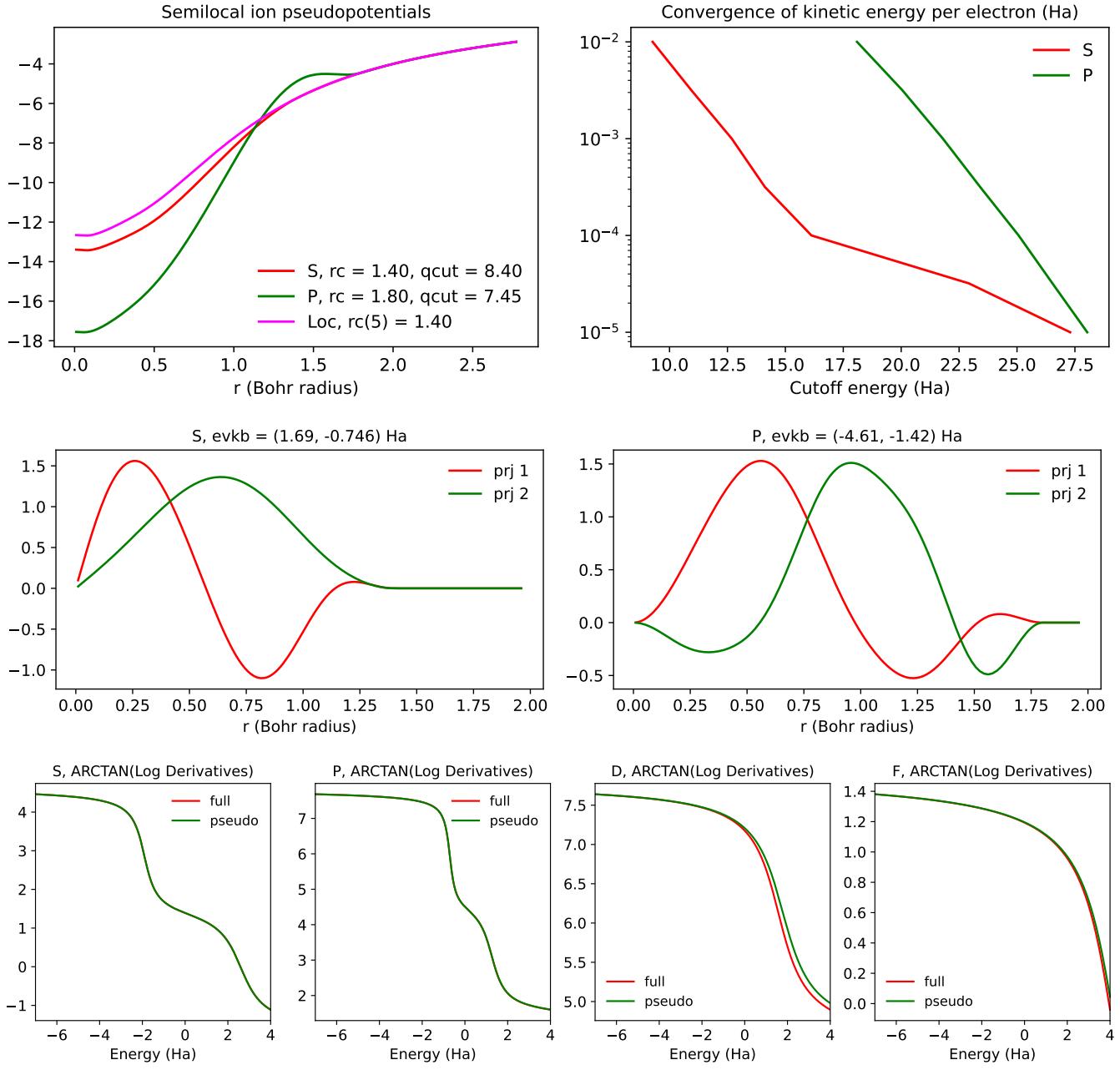
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 34                   | 38                   | 4.30                | 2.02     | 6.51      | 0.06                  | 0.67 | 0.16 | 0.26                  | 0.35 | 7.21              | 2.05 |
| PseudoDojo | 34                   | 38                   | 4.33                | 2.02     | 6.53      | 0.06                  | 0.67 | 0.18 | 0.57                  | 0.26 | 7.75              | 2.31 |
| SG15       | 36                   | 49                   | 3.09                | 0.35     | 1.10      | 0.03                  | 0.70 | 0.12 | 15.01                 | 7.35 | 2.99              | 0.64 |

# Fluorine (F)



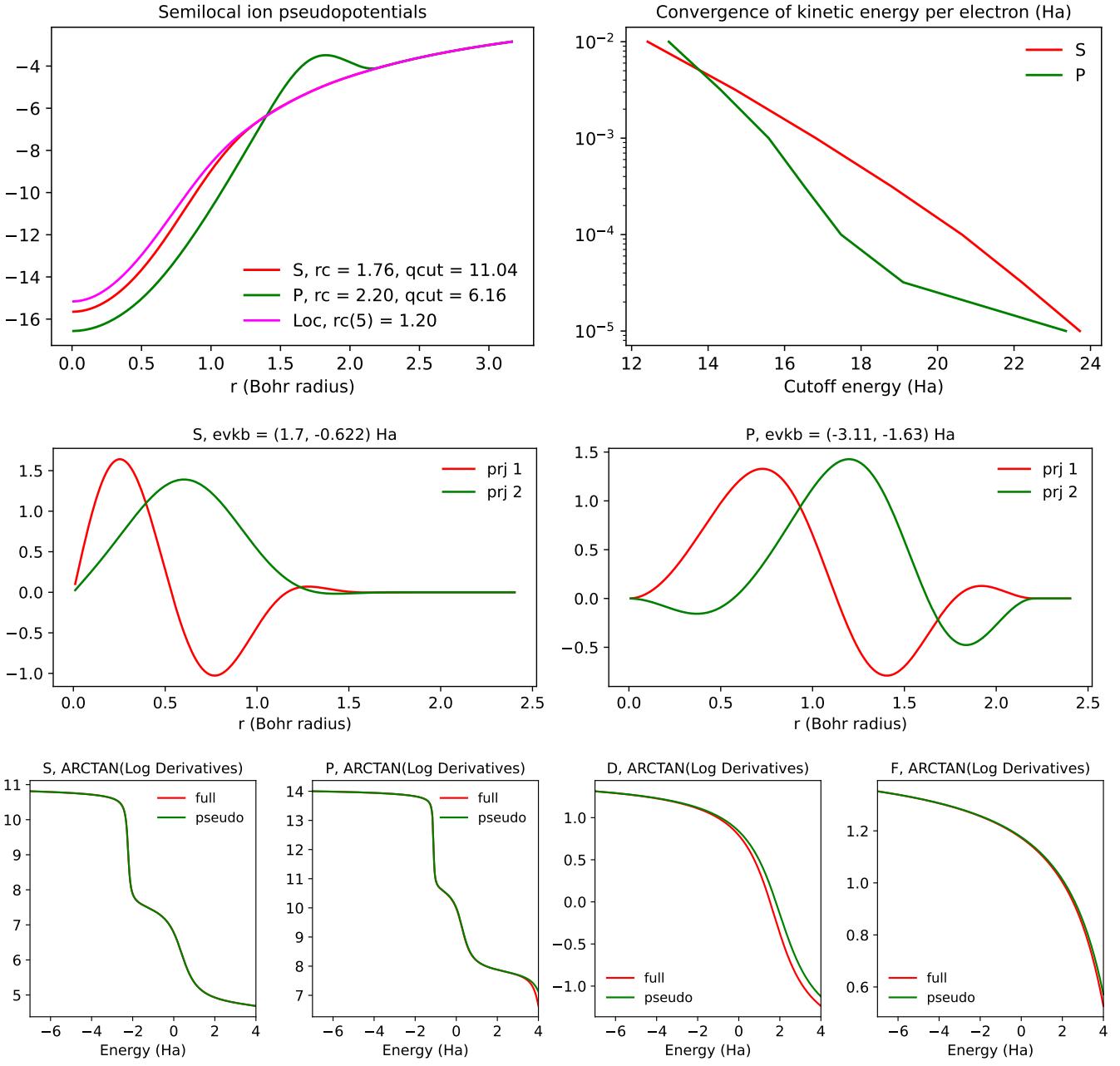
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 33                   | 37                   | 5.36                | 0.20     | 0.93      | 0.55                  | 0.92 | 0.29 | 0.14                  | 0.48 | 0.36              | 0.44 |
| PseudoDojo | 34                   | 39                   | 5.36                | 0.13     | 0.60      | 0.55                  | 0.92 | 0.26 | 0.03                  | 0.33 | 2.17              | 1.09 |
| SG15       | 32                   | 37                   | 4.94                | 0.90     | 4.09      | 0.51                  | 0.96 | 0.26 | 6.83                  | 5.85 | 10.31             | 1.18 |

# Neon (Ne)



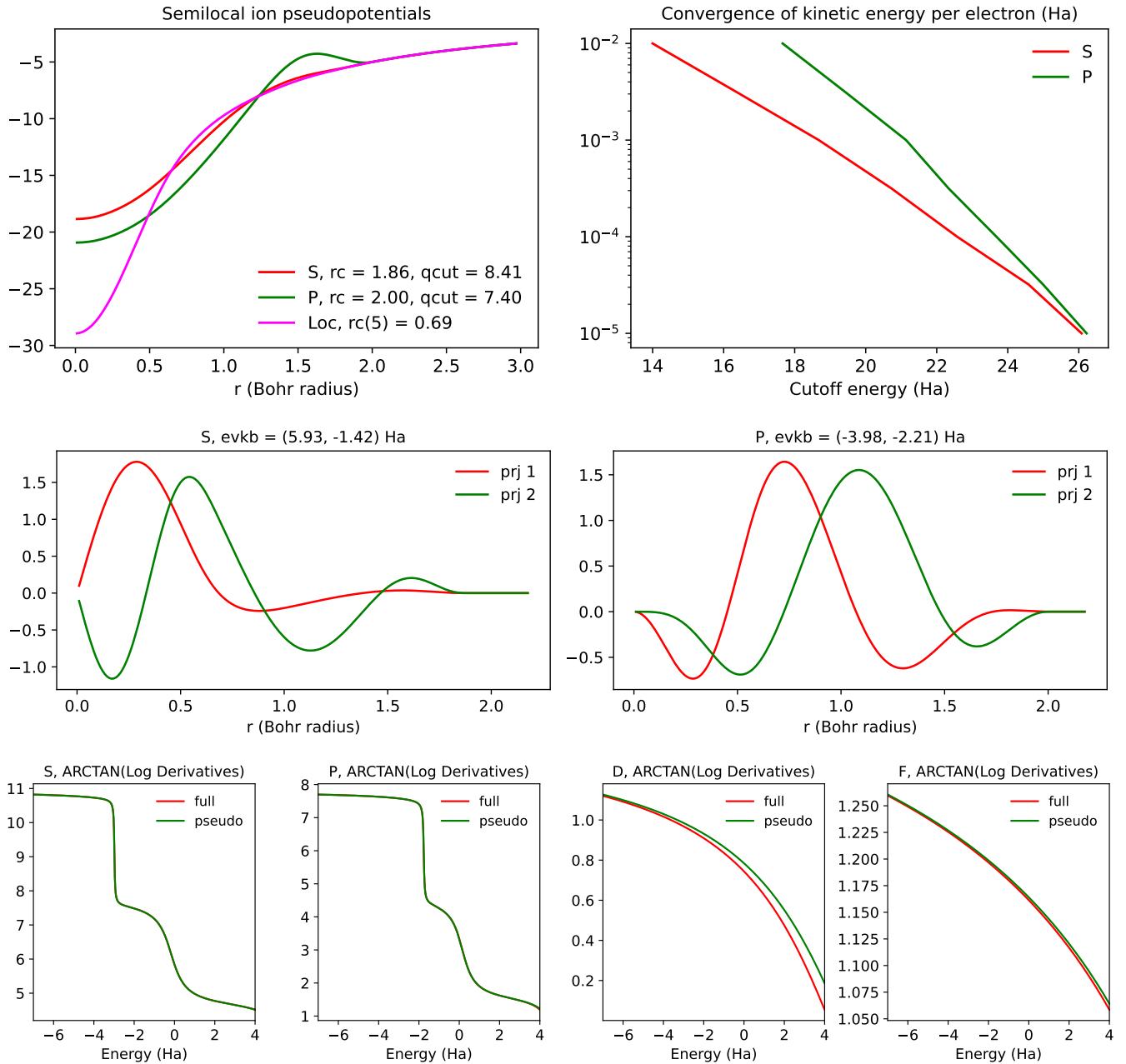
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |     |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |       |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|-----|------|-----------------------|------|-------------------|-------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC | COMP | LAP                   | HAP  | LOP               | HOP   |
| SPMS       | 24                   | 28                   | 0.65                | 0.03     | 2.56      | -                     | -   | -    | 2.03                  | 2.03 | 6.54              | 4.78  |
| PseudoDojo | 28                   | 32                   | 0.65                | 0.04     | 4.04      | -                     | -   | -    | 4.24                  | 4.24 | 5.94              | 4.41  |
| SG15       | 17                   | 19                   | 0.64                | 0.02     | 2.11      | -                     | -   | -    | 0.44                  | 0.44 | 32.05             | 25.28 |

# Sodium (Na)



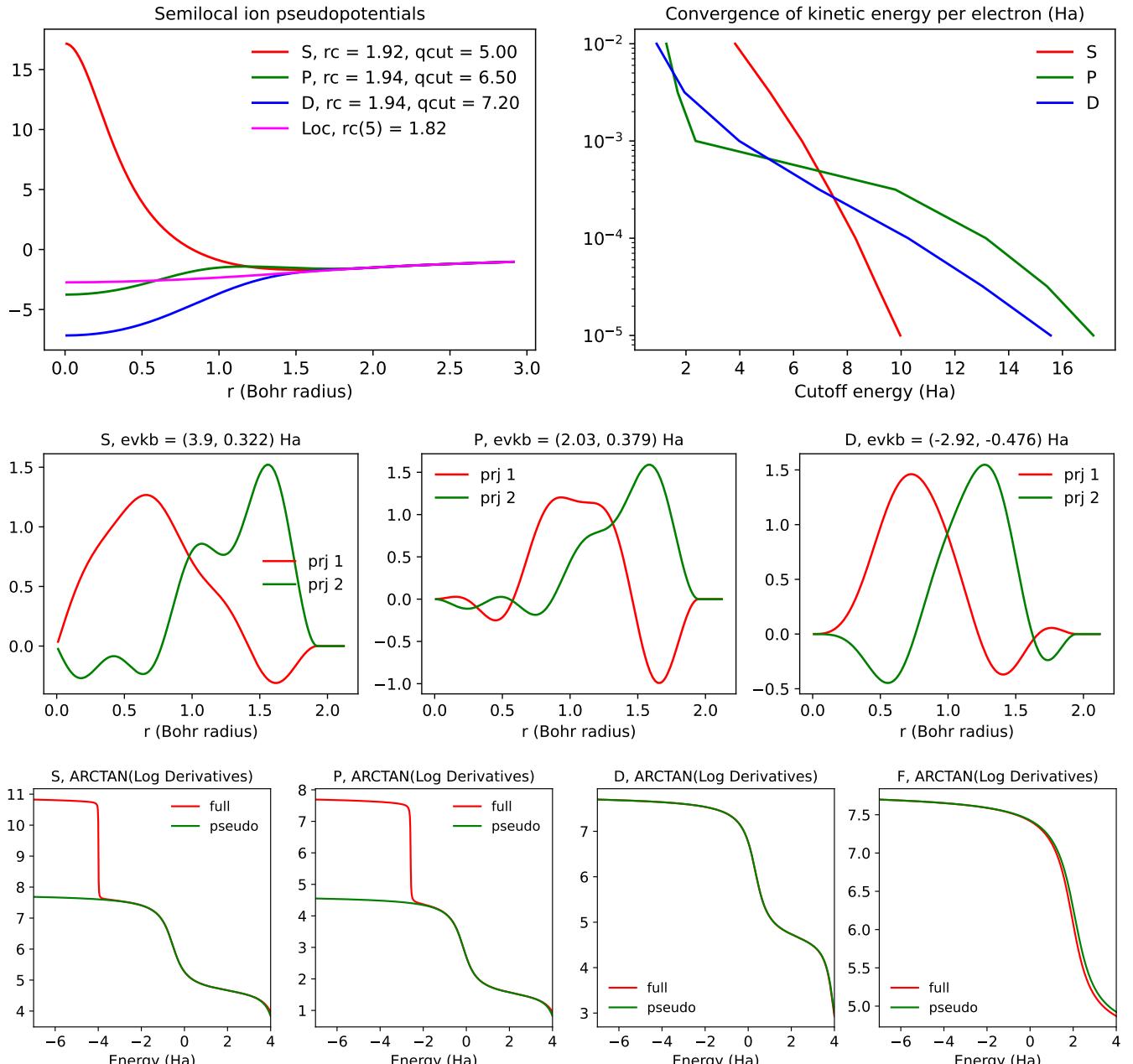
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 19                   | 24                   | 2.77                | 0.20     | 2.13      | 0.69                  | 0.69 | 0.24 | 0.22                  | 0.16 | 0.02              | 0.21 |
| PseudoDojo | 35                   | 39                   | 1.48                | 0.44     | 4.58      | 0.34                  | 0.34 | 0.09 | 0.20                  | 4.81 | 0.61              | 0.20 |
| SG15       | 29                   | 41                   | 1.48                | 0.41     | 4.27      | 0.36                  | 0.36 | 0.10 | 0.02                  | 0.17 | 0.05              | 0.06 |

# Magnesium (Mg)



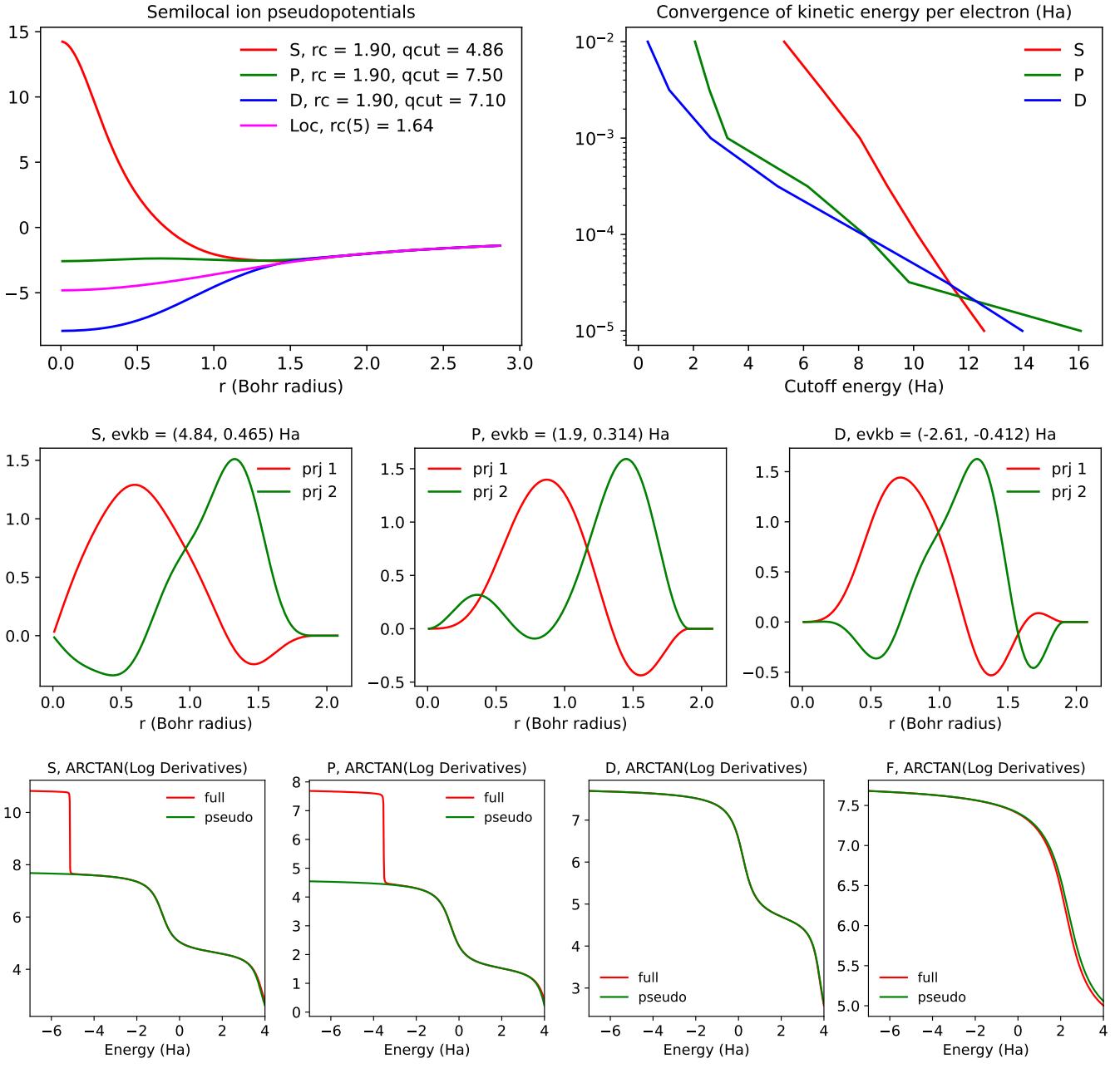
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 23                   | 28                   | 0.61                | 0.12     | 0.44      | 0.02                  | 0.02 | 0.11 | 0.16                  | 0.29 | 0.05              | 0.03 |
| PseudoDojo | 36                   | 39                   | 0.80                | 0.42     | 1.54      | 0.04                  | 0.04 | 0.07 | 2.91                  | 4.62 | 0.01              | 0.13 |
| SG15       | 28                   | 44                   | 0.91                | 0.42     | 1.51      | 0.04                  | 0.03 | 0.08 | 0.14                  | 0.61 | 0.00              | 0.02 |

# Aluminium (Al)



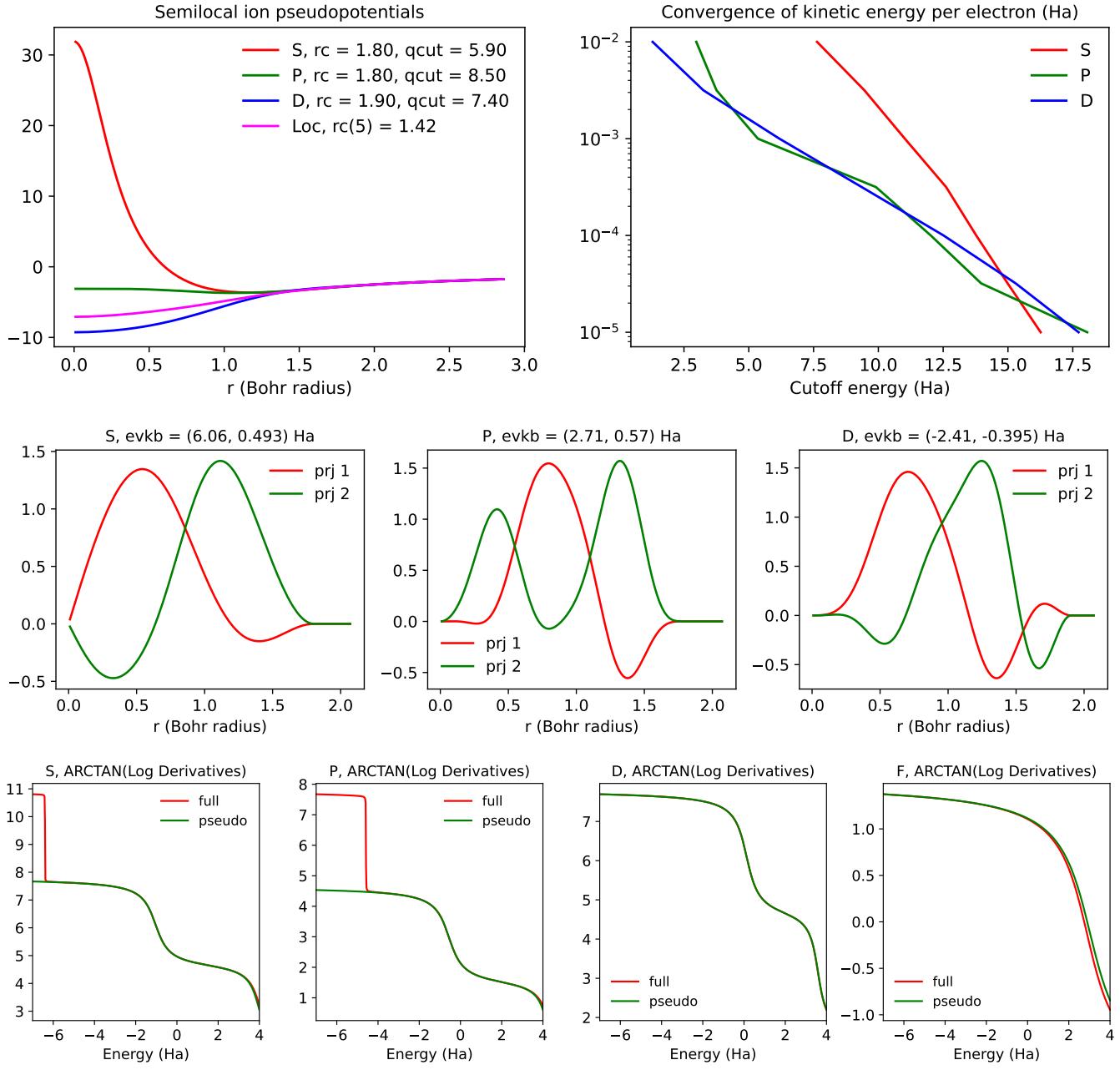
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 9                    | 14                   | 1.92                | 0.52     | 1.21      | 0.14                  | 0.14 | 0.07 | 0.16                  | 0.16 | 0.17              | 0.15 |
| PseudoDojo | 11                   | 17                   | 2.10                | 0.57     | 1.33      | 0.16                  | 0.15 | 0.08 | 0.12                  | 0.12 | 0.36              | 0.19 |
| SG15       | 29                   | 35                   | 1.45                | 1.04     | 2.44      | 0.05                  | 0.05 | 0.08 | -                     | -    | -                 | -    |

# Silicon (Si)



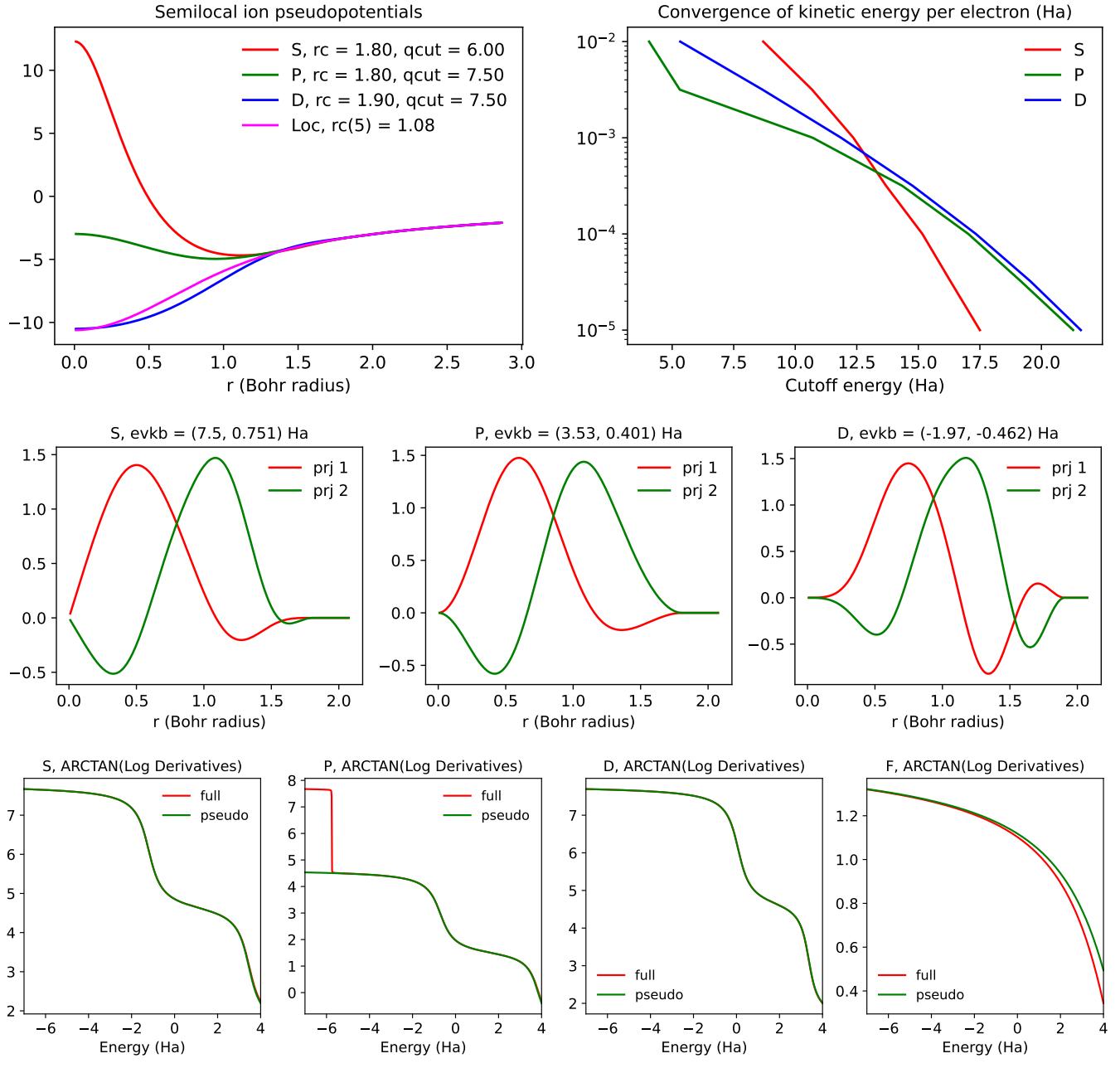
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 9                    | 15                   | 1.63                | 0.16     | 0.27      | 0.63                  | 0.24 | 0.10 | 1.51                  | 1.51 | 0.03              | 0.03 |
| PseudoDojo | 9                    | 15                   | 1.61                | 0.15     | 0.25      | 0.63                  | 0.24 | 0.09 | 1.50                  | 1.50 | 0.01              | 0.01 |
| SG15       | 11                   | 20                   | 1.14                | 1.69     | 2.82      | 0.68                  | 0.29 | 0.06 | 1.38                  | 1.38 | 0.01              | 0.01 |

# Phosphorus (P)



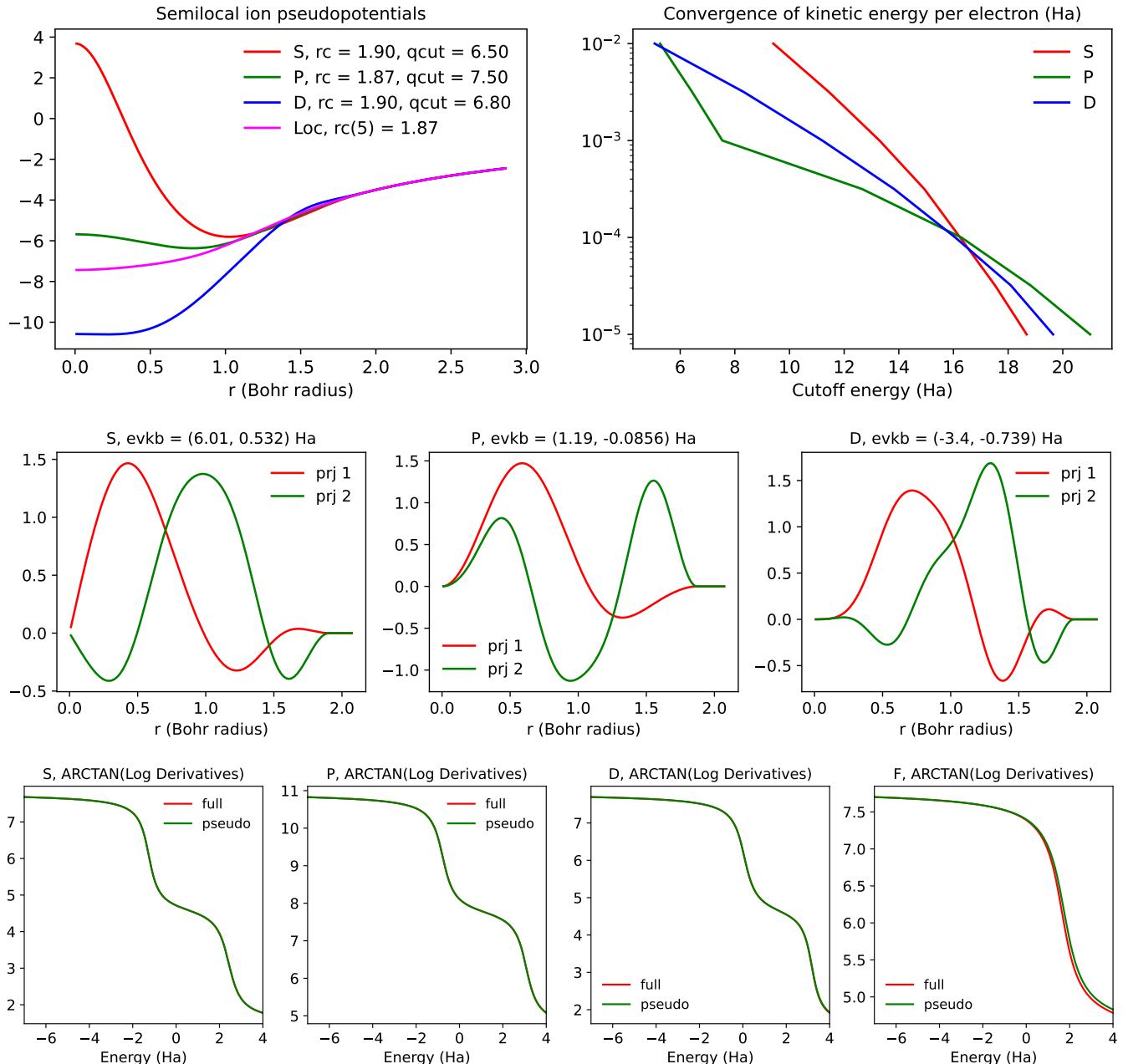
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 13                   | 17                   | 0.52                | 0.17     | 0.34      | 0.01                  | 0.00 | 0.08 | 0.08                  | 0.03 | 0.60              | 0.07 |
| PseudoDojo | 13                   | 18                   | 0.57                | 0.15     | 0.31      | 0.01                  | 0.01 | 0.05 | 0.08                  | 0.02 | 1.62              | 0.03 |
| SG15       | 18                   | 29                   | 0.74                | 0.05     | 0.10      | 0.02                  | 0.01 | 0.03 | 0.06                  | 0.15 | 0.57              | 0.08 |

# Sulfur (S)



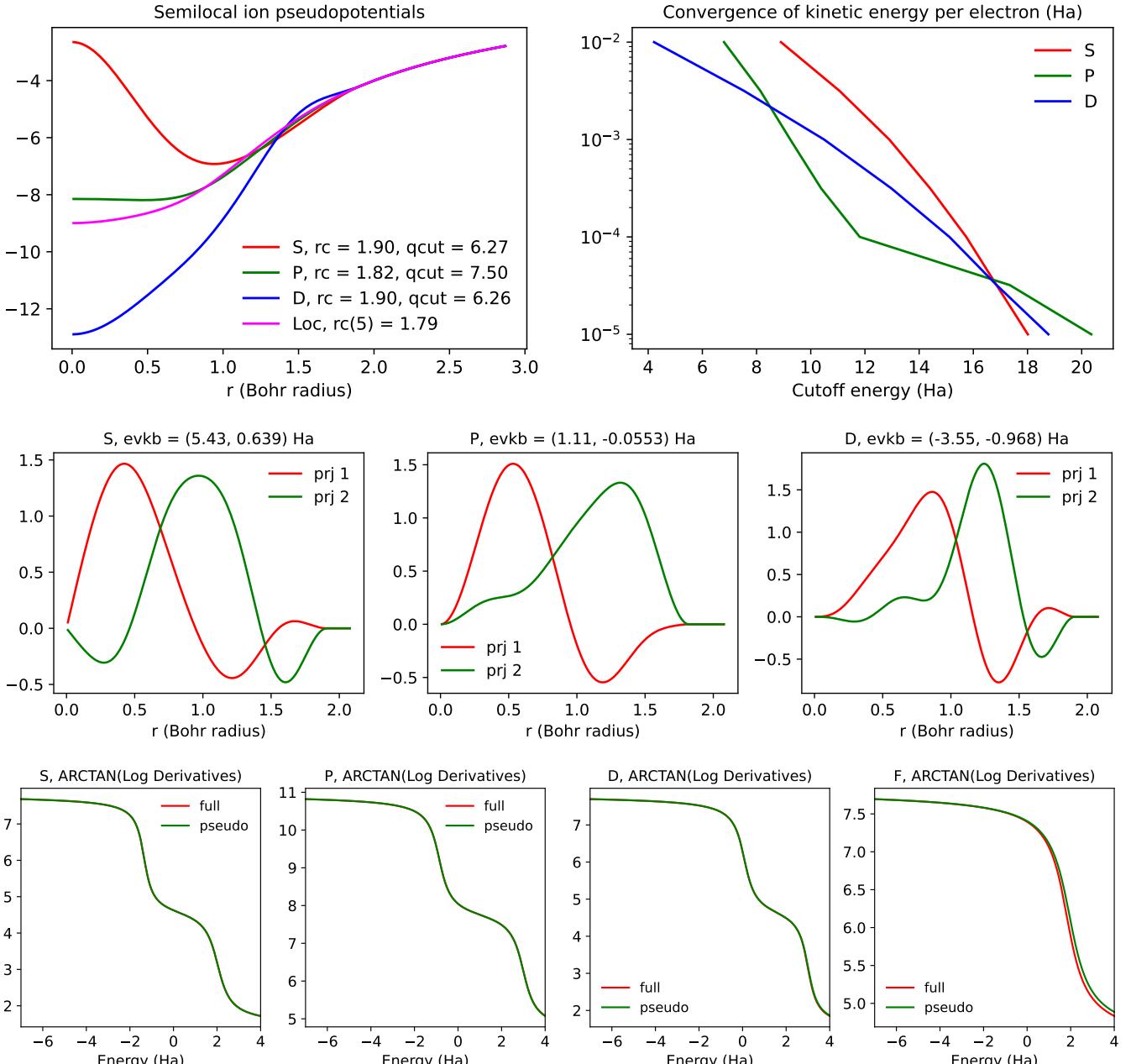
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |     |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|-----|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP |
| SPMS       | 15                   | 20                   | 1.02                | 0.01     | 0.02      | 0.07                  | 0.15 | 0.08 | 0.17                  | 0.22 | -                 | -   |
| PseudoDojo | 16                   | 20                   | 1.04                | 0.04     | 0.08      | 0.07                  | 0.15 | 0.09 | 0.24                  | 0.26 | -                 | -   |
| SG15       | 18                   | 33                   | 4.15                | 1.80     | 3.74      | 0.27                  | 0.33 | 0.09 | 0.66                  | 3.05 | -                 | -   |

# Chlorine (Cl)



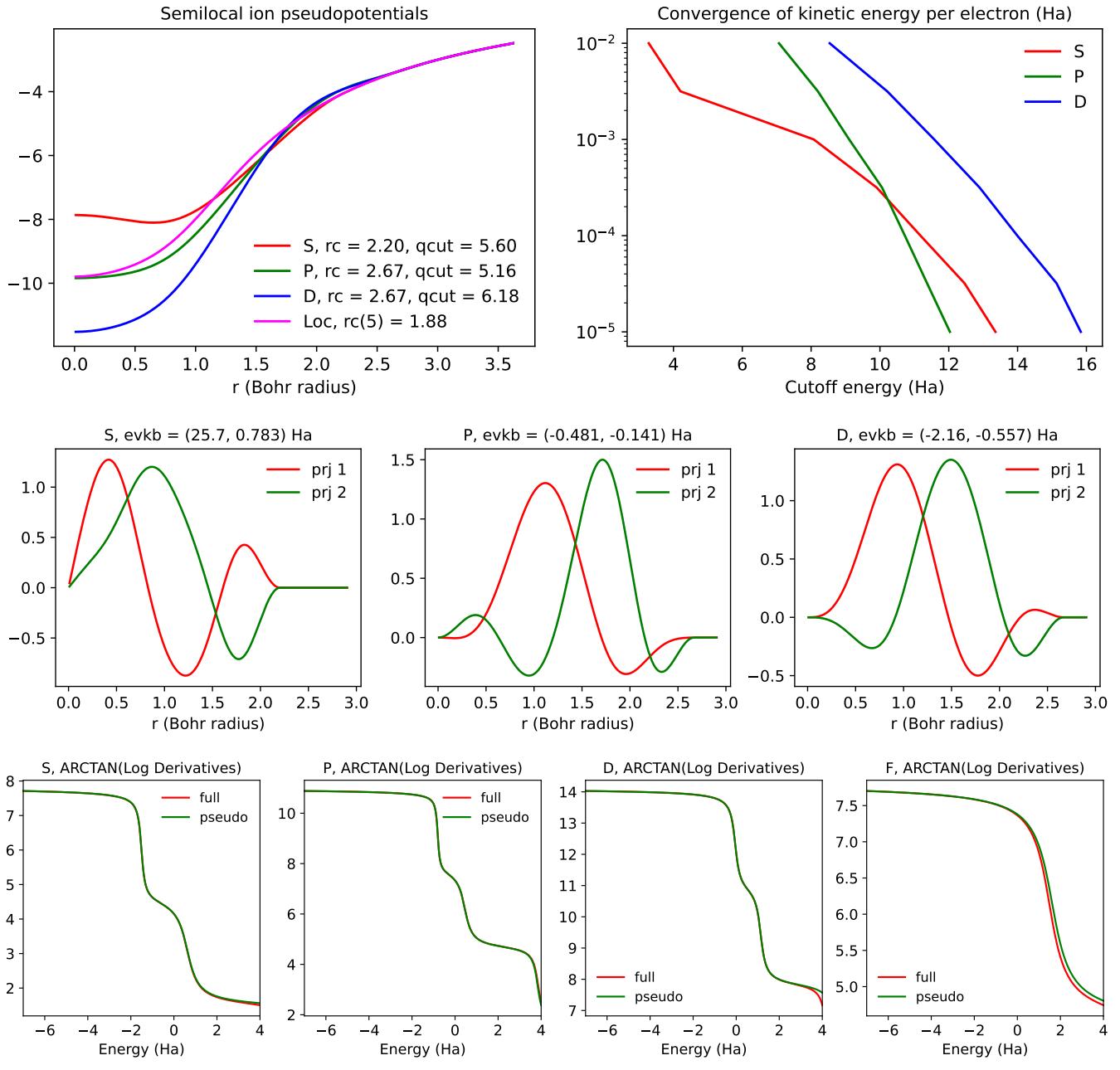
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 16                   | 20                   | 8.62                | 0.14     | 0.59      | 2.31                  | 0.36 | 0.29 | 0.11                  | 0.18 | 2.08              | 2.32 |
| PseudoDojo | 20                   | 25                   | 3.71                | 0.75     | 3.08      | 2.30                  | 0.38 | 0.25 | 0.17                  | 0.23 | 2.71              | 3.21 |
| SG15       | 18                   | 31                   | 48.06               | 1.81     | 7.36      | 2.59                  | 0.08 | 0.25 | 0.35                  | 0.34 | 0.82              | 0.50 |

# Argon (Ar)



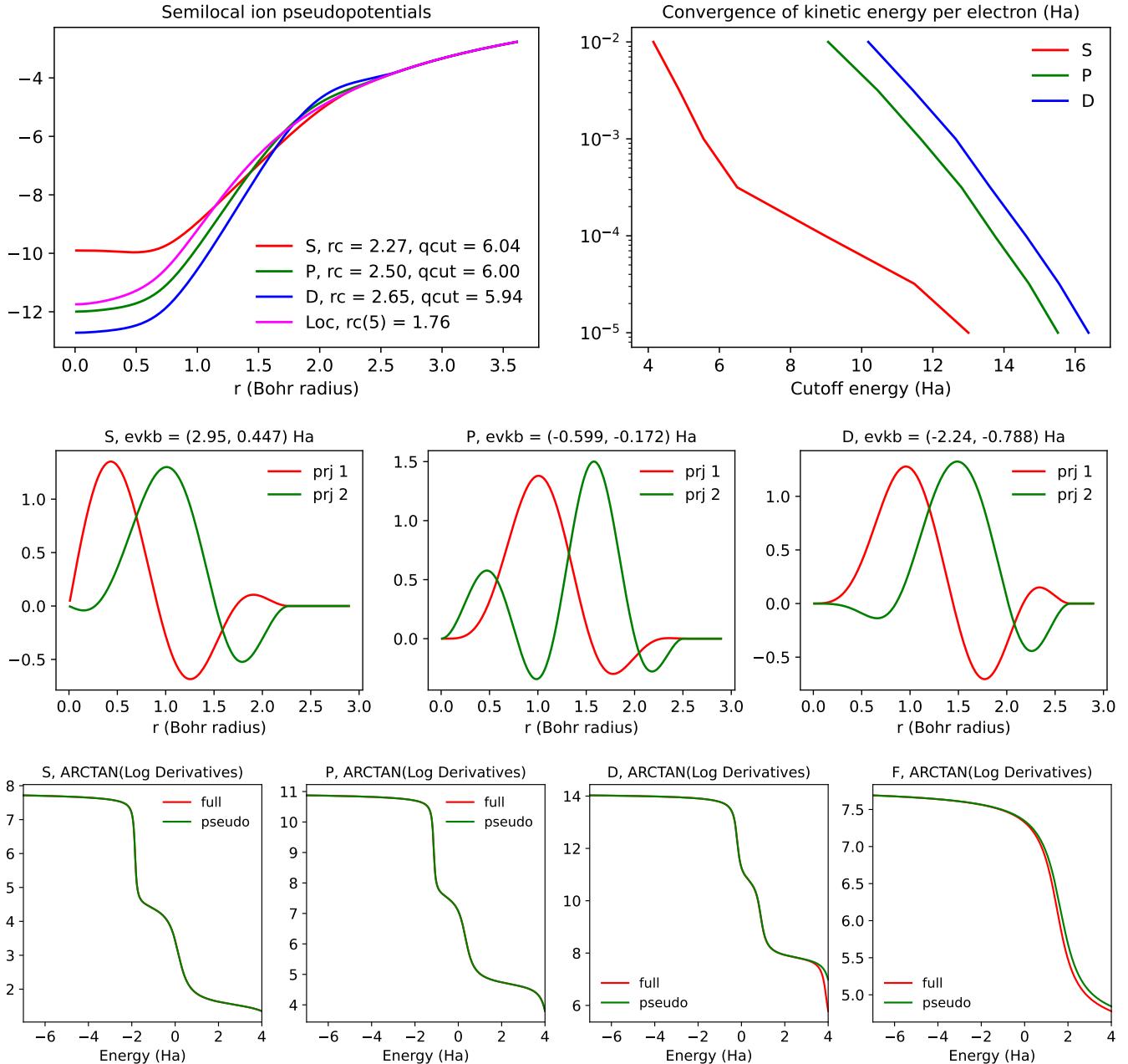
|            | $E_{cut}$            |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{lat}$ |     |      | $\delta_{asr}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|----------------|-----|------|----------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC            | FCC | COMP | LAP            | HAP  | LOP               | HOP  |
| SPMS       | 14                   | 19                   | 0.90                | 0.02     | 1.16      | -              | -   | -    | 0.29           | 0.29 | 2.62              | 2.74 |
| PseudoDojo | 23                   | 28                   | 0.90                | 0.02     | 1.18      | -              | -   | -    | 0.22           | 0.22 | 1.55              | 0.91 |
| SG15       | 19                   | 24                   | 0.91                | 0.02     | 1.65      | -              | -   | -    | 0.23           | 0.23 | 1.03              | 0.54 |

# Potassium (K)



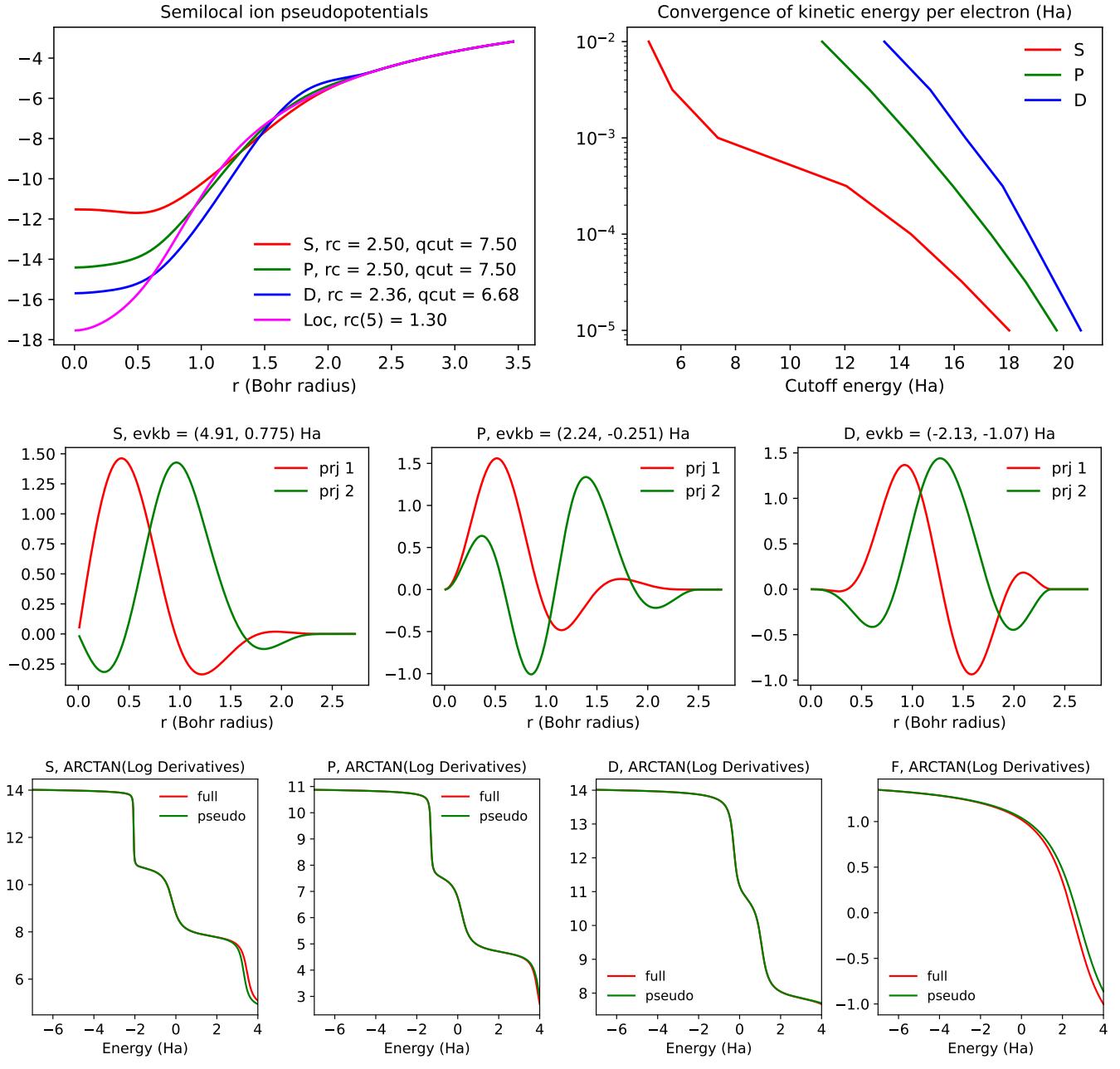
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 11                   | 13                   | 0.36                | 0.18     | 2.03      | 0.05                  | 0.06 | 0.23 | 0.24                  | 0.24 | 0.05              | 0.05 |
| PseudoDojo | 27                   | 32                   | 0.36                | 0.18     | 2.02      | 0.05                  | 0.06 | 0.21 | 0.43                  | 0.43 | 0.02              | 0.02 |
| SG15       | 14                   | 17                   | 0.37                | 0.17     | 1.99      | 0.05                  | 0.07 | 0.21 | 1.49                  | 1.49 | 0.08              | 0.08 |

# Calcium (Ca)



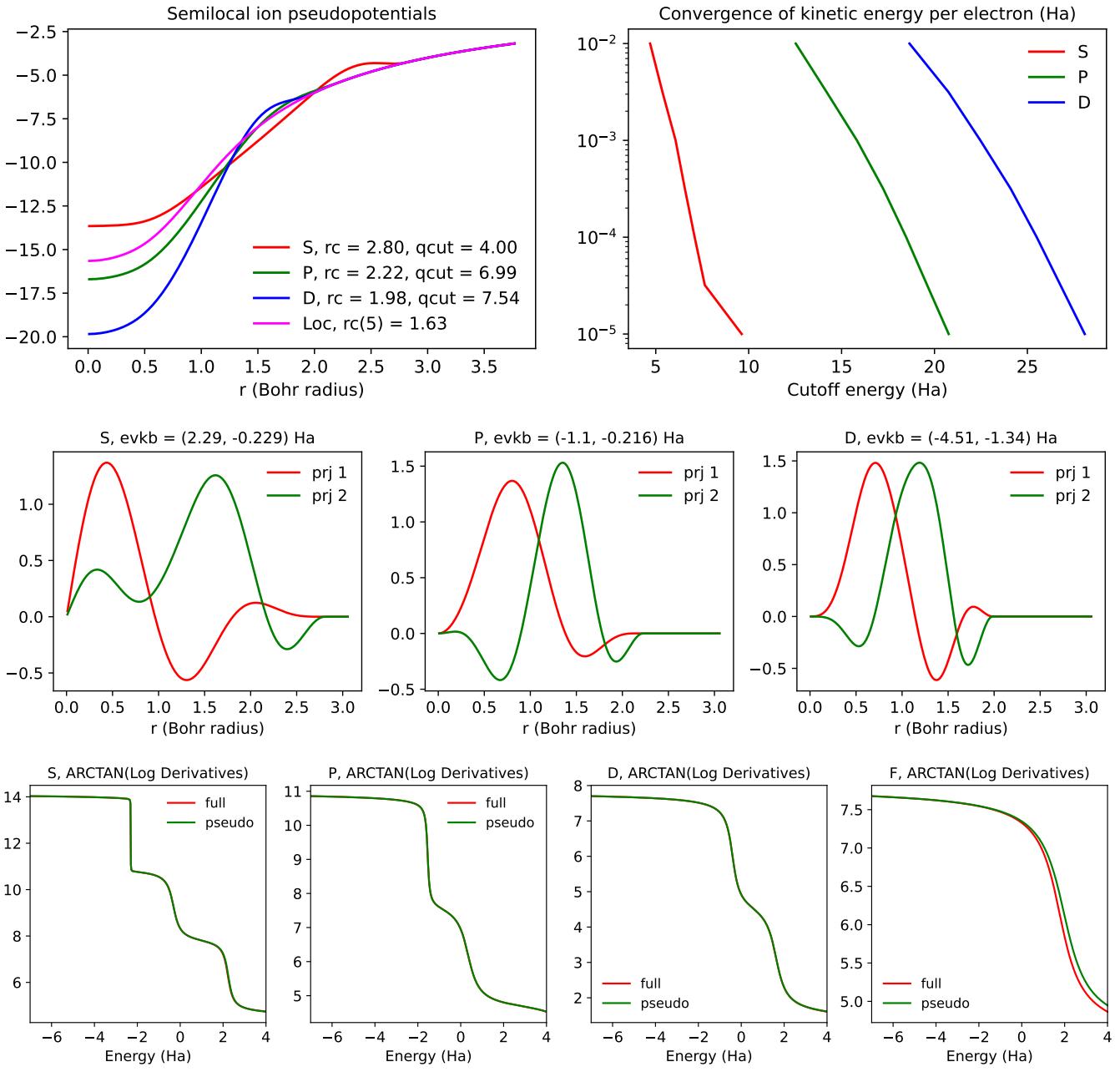
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 13                   | 16                   | 0.79                | 0.39     | 1.60      | 0.03                  | 0.08 | 0.09 | 0.53                  | 0.53 | 0.02              | 0.00 |
| PseudoDojo | 26                   | 31                   | 1.24                | 0.06     | 0.26      | 0.13                  | 0.15 | 0.08 | 1.62                  | 1.62 | 0.00              | 0.02 |
| SG15       | 17                   | 20                   | 1.06                | 0.11     | 0.45      | 0.11                  | 0.14 | 0.07 | 1.06                  | 1.06 | 0.22              | 0.12 |

# Scandium (Sc)



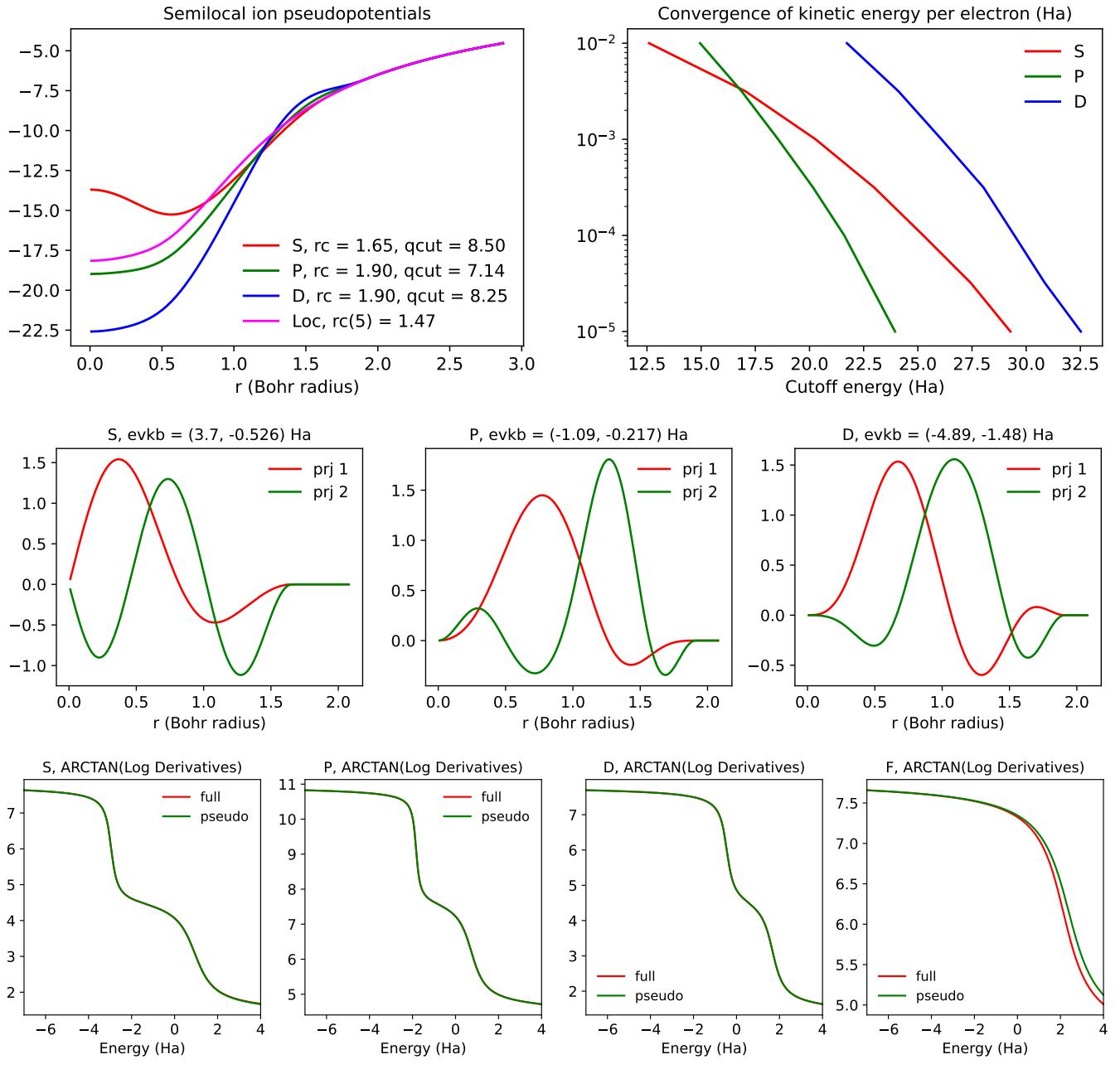
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |       | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|-------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP   | LOP               | HOP  |
| SPMS       | 17                   | 20                   | 4.43                | 1.25     | 2.84      | 0.11                  | 0.13 | 0.06 | 16.41                 | 11.61 | 0.03              | 0.13 |
| PseudoDojo | 31                   | 36                   | 2.87                | 1.26     | 2.85      | 0.12                  | 0.12 | 0.06 | 17.11                 | 12.09 | 0.04              | 0.05 |
| SG15       | 17                   | 20                   | 4.39                | 1.48     | 3.35      | 0.09                  | 0.10 | 0.05 | 0.29                  | 0.33  | 0.03              | 0.08 |

# Titanium (Ti)



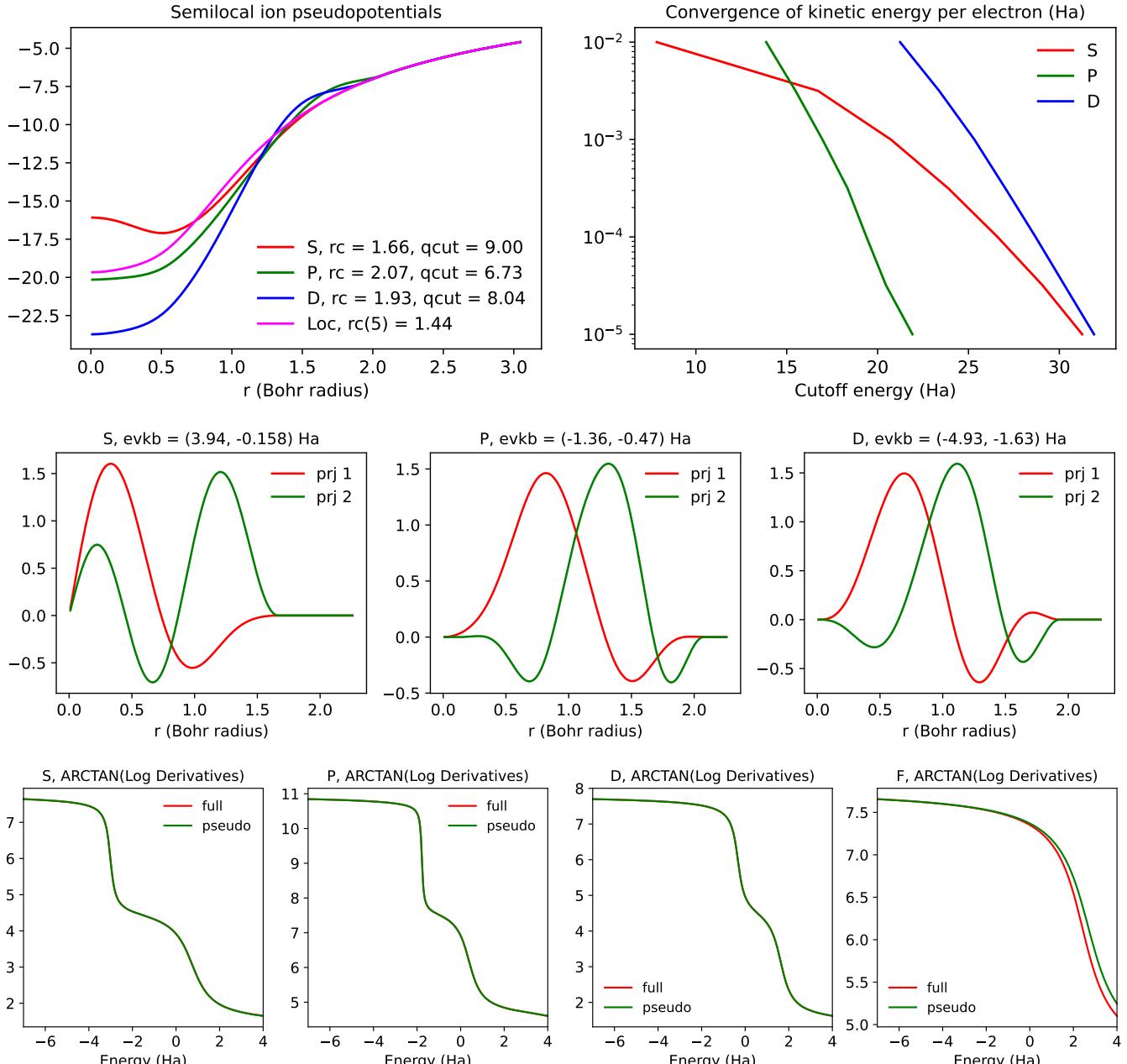
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 23                   | 26                   | 4.12                | 1.05     | 1.63      | 0.00                  | 0.00 | 0.07 | 9.63                  | 6.80 | 0.27              | 0.36 |
| PseudoDojo | 33                   | 38                   | 2.10                | 0.86     | 1.33      | 0.02                  | 0.01 | 0.08 | 10.59                 | 7.50 | 0.04              | 0.11 |
| SG15       | 21                   | 26                   | 5.28                | 1.07     | 1.67      | 0.00                  | 0.01 | 0.06 | 0.23                  | 0.47 | 0.01              | 0.01 |

# Vanadium (V)



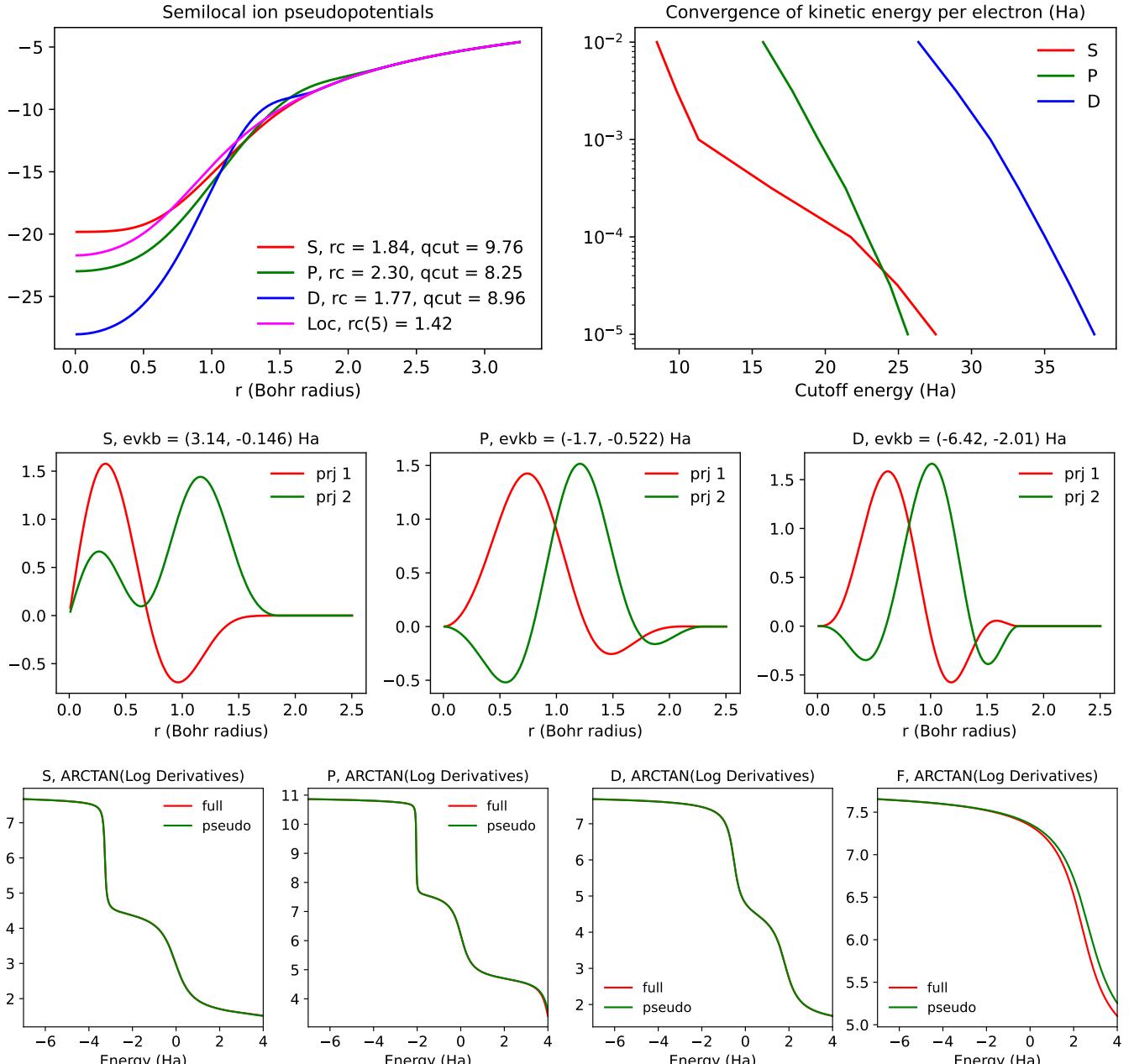
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 27                   | 31                   | 2.64                | 1.75     | 2.15      | 0.00                  | 0.02 | 0.11 | 0.07                  | 0.07 | 0.20              | 0.20 |
| PseudoDojo | 34                   | 39                   | 2.14                | 1.34     | 1.64      | 0.03                  | 0.01 | 0.10 | 0.22                  | 0.22 | 0.00              | 0.00 |
| SG15       | 28                   | 49                   | 2.60                | 1.82     | 2.23      | 0.00                  | 0.02 | 0.06 | 2.77                  | 2.77 | 0.02              | 0.02 |

# Chromium (Cr)



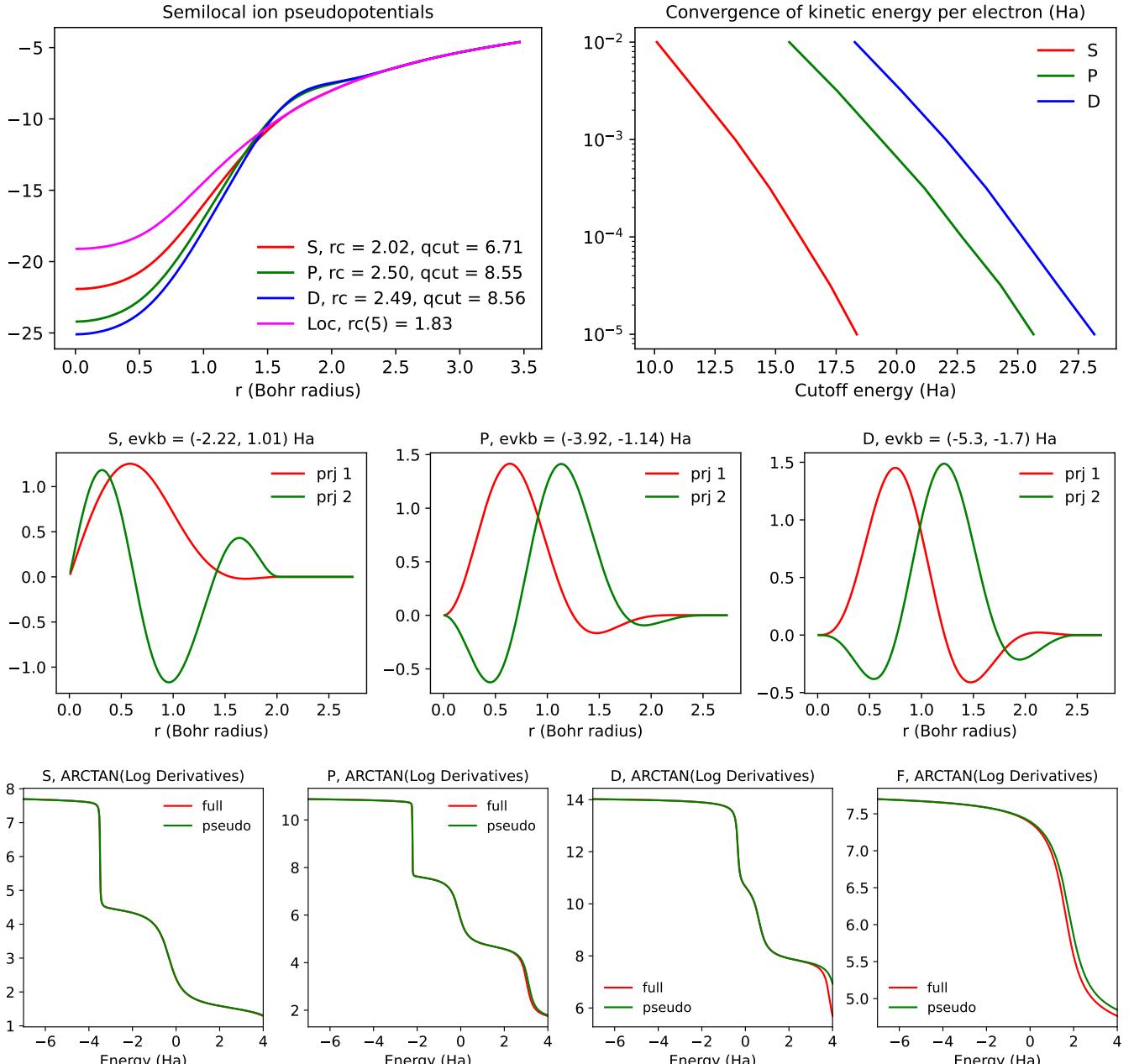
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 27                   | 32                   | 3.74                | 11.65    | 19.80     | 0.30                  | 0.24 | 0.09 | 0.34                  | 0.34 | 0.02              | 0.02 |
| PseudoDojo | 39                   | 43                   | 3.00                | 10.50    | 18.15     | 0.16                  | 0.10 | 0.12 | 0.20                  | 0.20 | 0.15              | 0.15 |
| SG15       | 22                   | 25                   | 5.34                | 20.75    | 43.53     | 0.27                  | 0.21 | 0.02 | 0.41                  | 0.41 | 0.06              | 0.06 |

# Manganese (Mn)



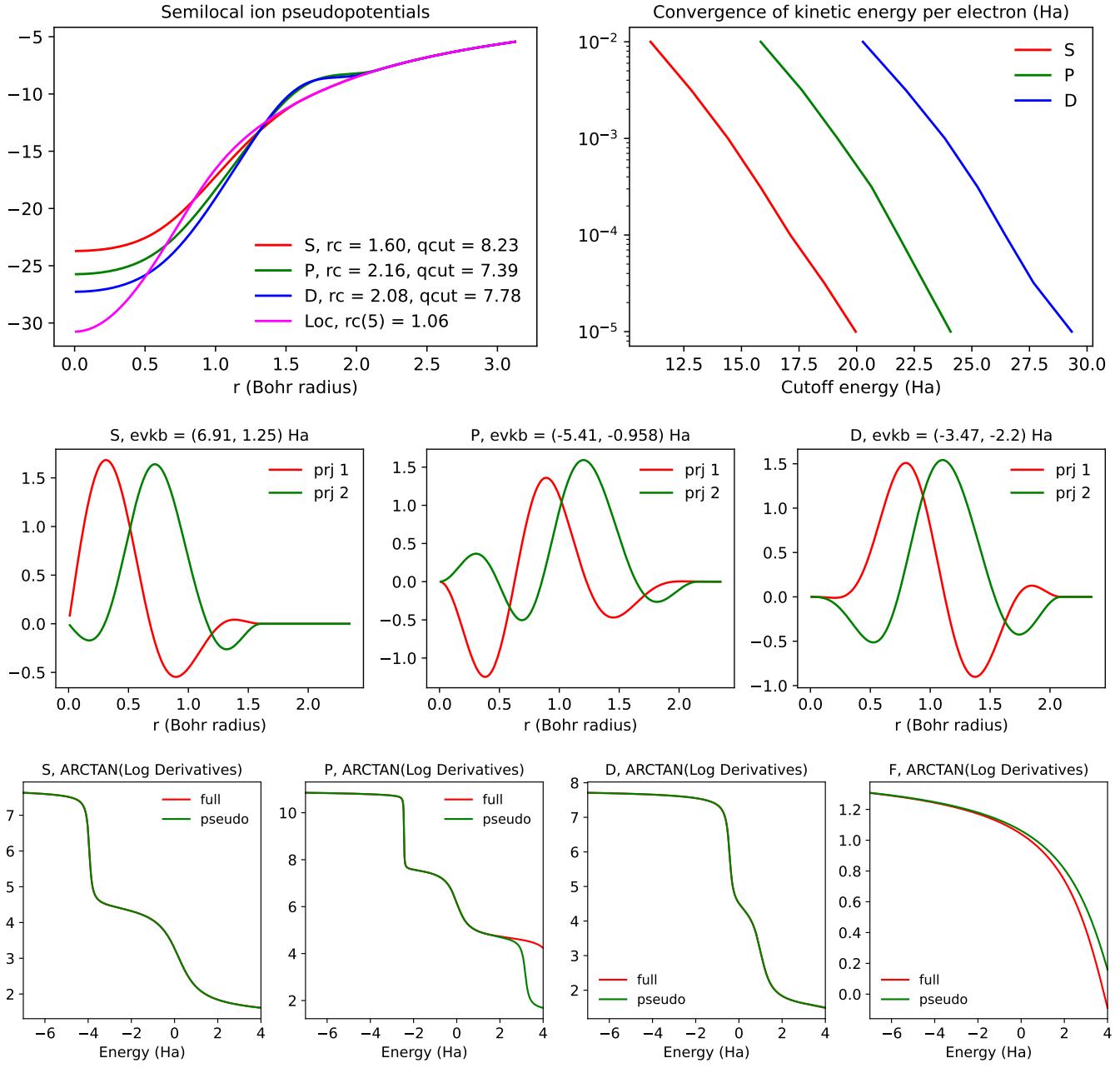
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 33                   | 37                   | 2.23                | 7.75     | 16.33     | 0.16                  | 0.14 | 0.08 | 0.13                  | 0.18 | 0.23              | 0.15 |
| PseudoDojo | 41                   | 45                   | 2.71                | 8.03     | 16.95     | 0.10                  | 0.08 | 0.10 | 0.16                  | 0.43 | 0.13              | 0.09 |
| SG15       | 27                   | 38                   | 4.82                | 12.90    | 26.71     | 0.20                  | 0.17 | 0.07 | 0.27                  | 0.58 | 0.04              | 0.02 |

# Iron (Fe)



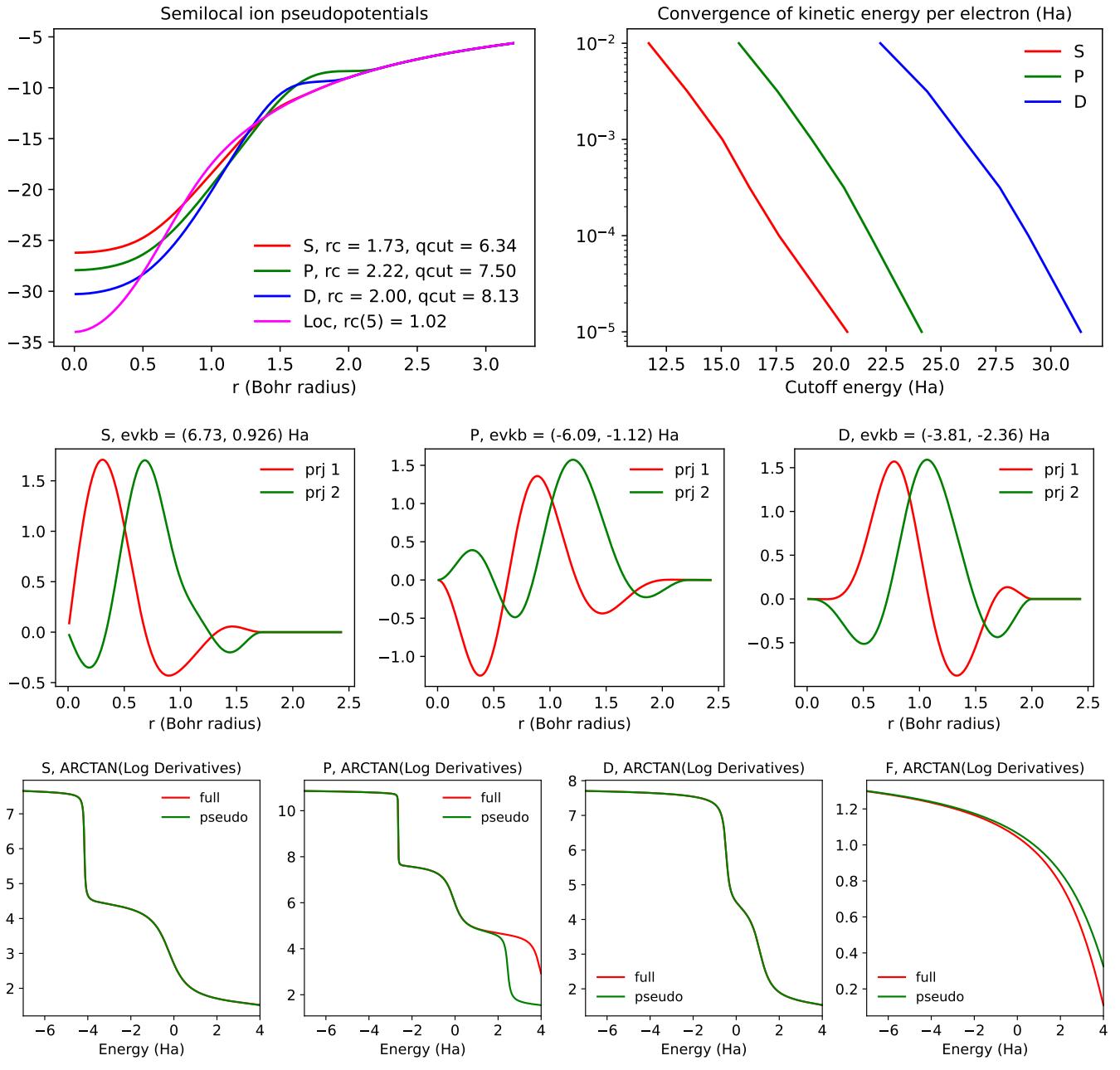
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 25                   | 32                   | 3.93                | 6.12     | 9.75      | 0.11                  | 0.10 | 0.09 | 0.30                  | 0.30 | 0.00              | 0.00 |
| PseudoDojo | 40                   | 44                   | 4.73                | 5.60     | 9.22      | 0.06                  | 0.02 | 0.08 | 0.56                  | 0.56 | 0.02              | 0.02 |
| SG15       | 31                   | 34                   | 3.12                | 5.85     | 9.19      | 0.17                  | 0.14 | 0.04 | 0.79                  | 0.79 | 0.05              | 0.05 |

# Cobalt (Co)



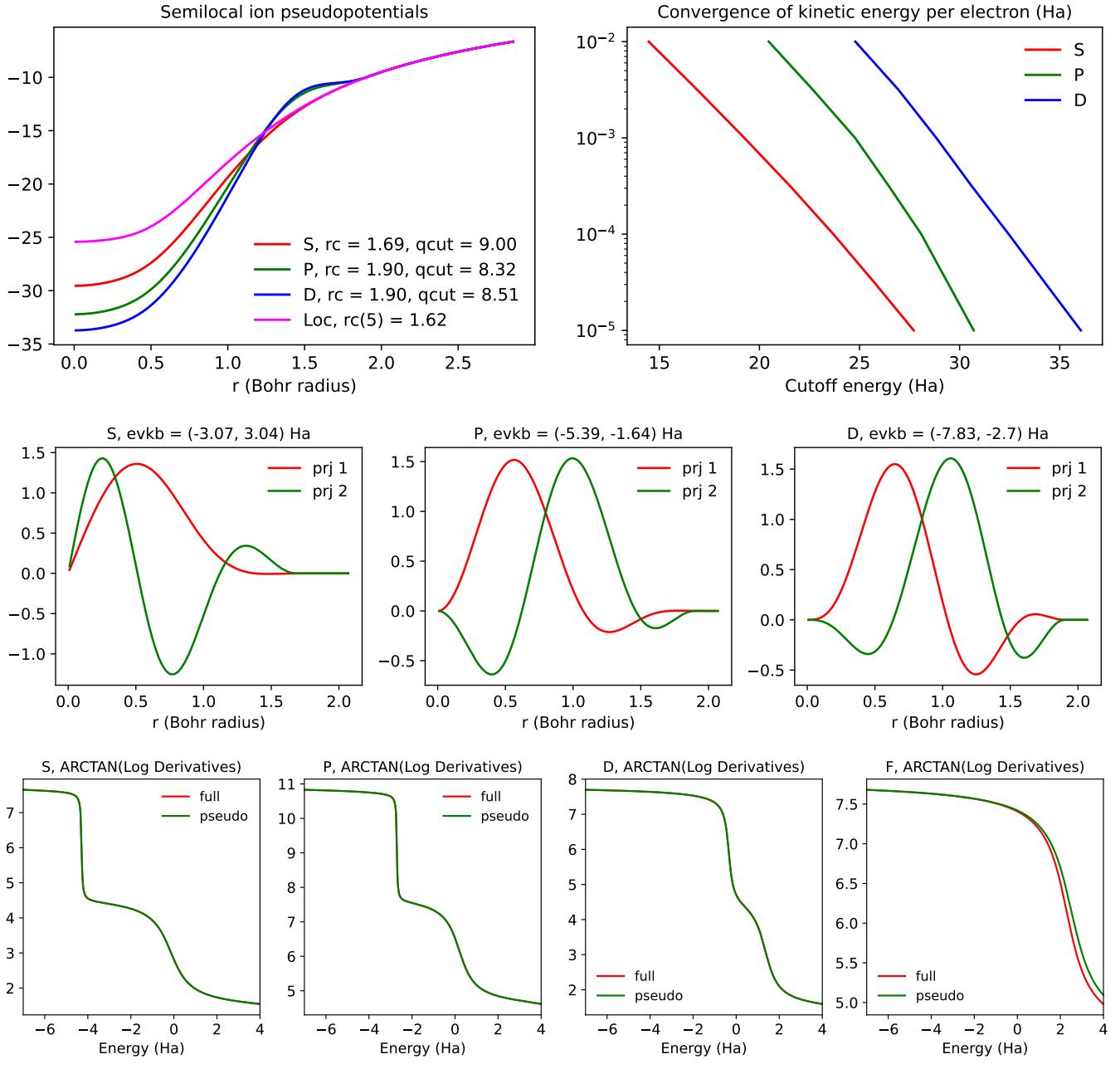
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |       | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|-------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP   | LOP               | HOP  |
| SPMS       | 26                   | 31                   | 3.43                | 0.33     | 0.44      | 0.06                  | 0.06 | 0.09 | 24.73                 | 17.49 | 0.01              | 0.13 |
| PseudoDojo | 41                   | 47                   | 1.55                | 1.06     | 1.38      | 0.01                  | 0.02 | 0.07 | 43.00                 | 30.41 | 0.00              | 0.04 |
| SG15       | 27                   | 33                   | 6.76                | 3.56     | 4.68      | 0.14                  | 0.14 | 0.05 | 0.38                  | 0.62  | 0.01              | 0.03 |

# Nickel (Ni)



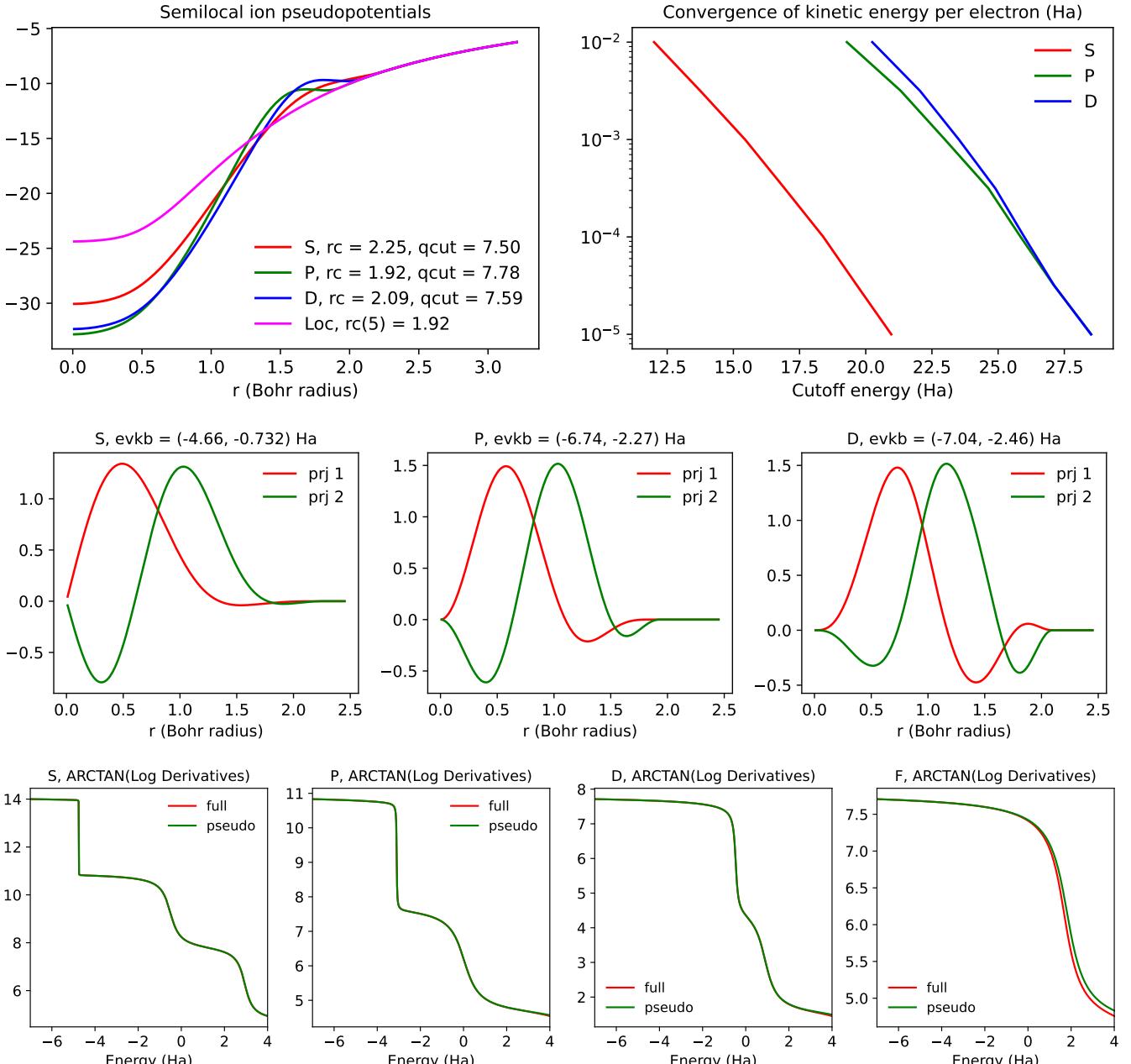
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 29                   | 34                   | 2.93                | 0.54     | 0.76      | 0.10                  | 0.10 | 0.09 | 0.15                  | 0.15 | 0.05              | 0.07 |
| PseudoDojo | 42                   | 47                   | 1.32                | 1.07     | 1.50      | 0.08                  | 0.08 | 0.07 | 0.46                  | 0.46 | 0.01              | 0.02 |
| SG15       | 28                   | 31                   | 7.66                | 3.28     | 4.65      | 0.10                  | 0.10 | 0.06 | 0.38                  | 0.38 | 0.08              | 0.04 |

# Copper (Cu)



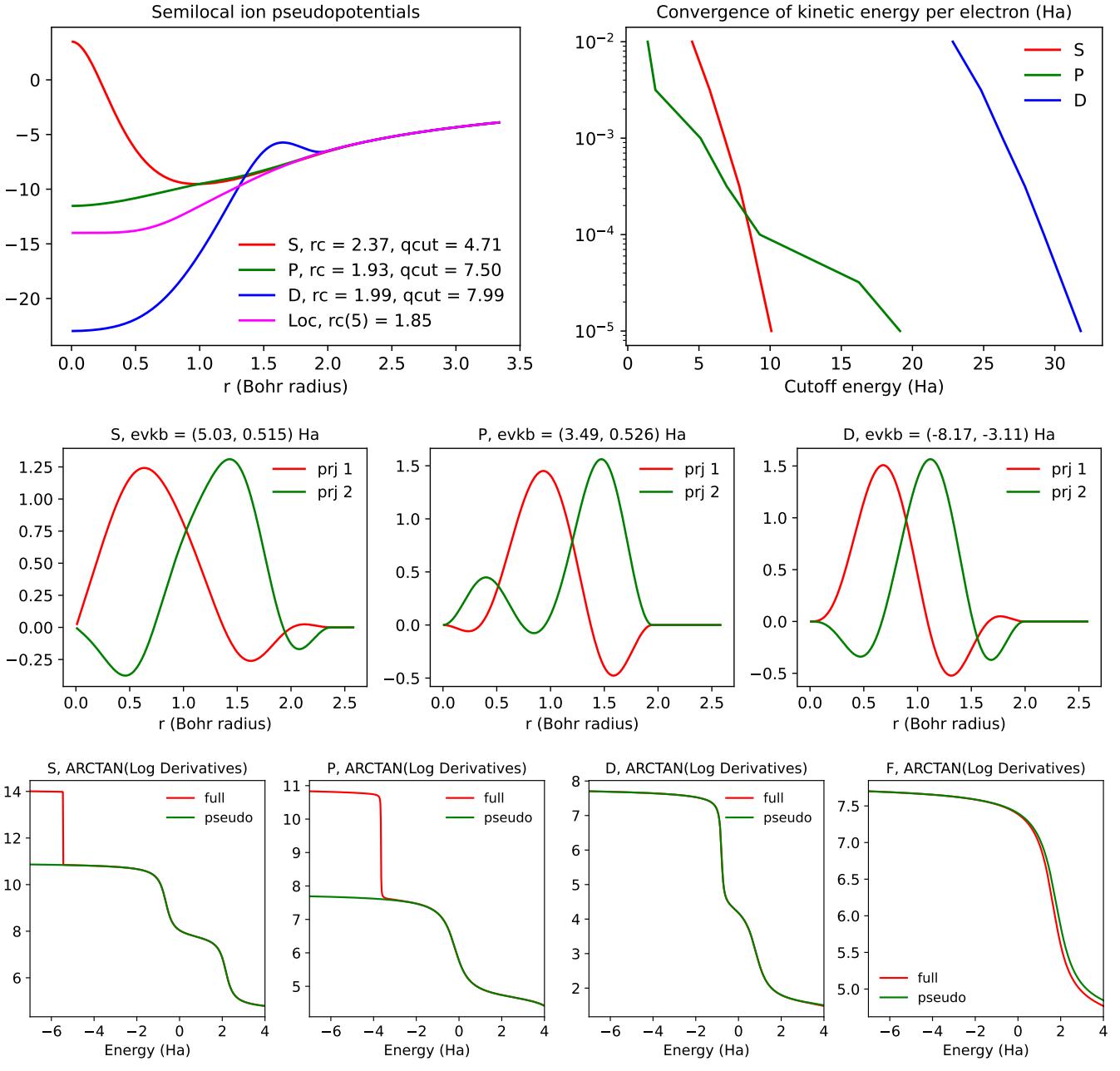
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 32                   | 35                   | 3.05                | 0.31     | 0.54      | 0.11                  | 0.06 | 0.07 | 0.52                  | 0.52 | 0.00              | 0.03 |
| PseudoDojo | 40                   | 44                   | 2.85                | 0.53     | 0.93      | 0.17                  | 0.12 | 0.07 | 0.71                  | 0.71 | 0.00              | 0.01 |
| SG15       | 37                   | 58                   | 2.52                | 1.04     | 1.88      | 0.04                  | 0.02 | 0.08 | 0.54                  | 0.54 | 0.01              | 0.01 |

# Zinc (Zn)



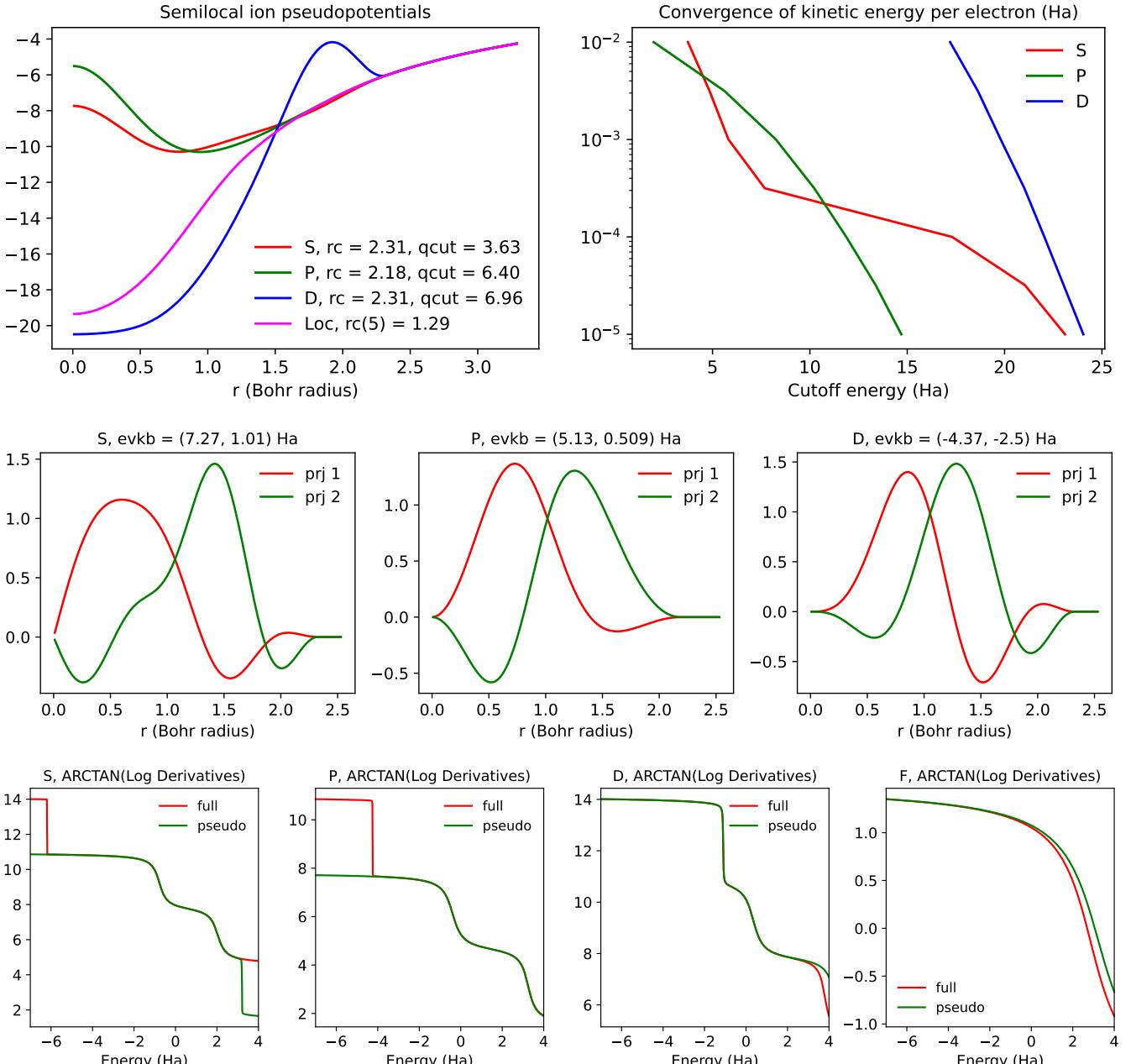
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |       | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|-------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP   | LOP               | HOP  |
| SPMS       | 27                   | 30                   | 0.34                | 0.80     | 2.11      | 0.04                  | 0.03 | 0.12 | 39.60                 | 28.00 | 0.09              | 0.00 |
| PseudoDojo | 36                   | 39                   | 1.32                | 0.29     | 0.78      | 0.16                  | 0.16 | 0.12 | 62.04                 | 43.86 | 0.04              | 0.04 |
| SG15       | 32                   | 51                   | 1.36                | 0.16     | 0.42      | 0.15                  | 0.15 | 0.10 | 0.06                  | 0.30  | 0.01              | 0.02 |

# Gallium (Ga)



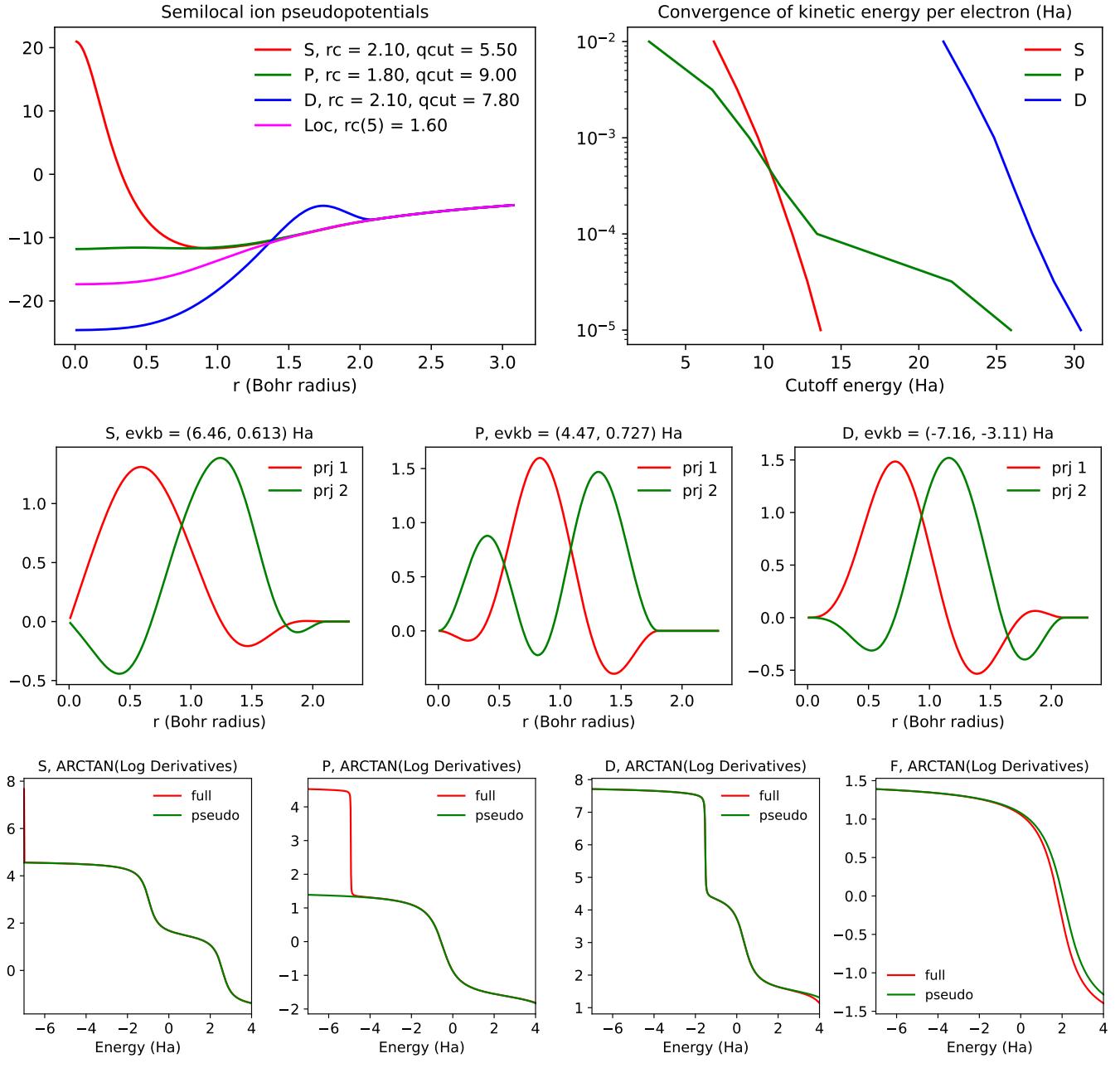
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 29                   | 34                   | 0.65                | 0.97     | 2.94      | 0.03                  | 0.01 | 0.06 | 0.04                  | 0.07 | 0.09              | 0.04 |
| PseudoDojo | 35                   | 39                   | 0.97                | 0.50     | 1.51      | 0.09                  | 0.07 | 0.08 | 0.06                  | 0.06 | 0.13              | 0.42 |
| SG15       | 55                   | 63                   | 0.91                | 0.62     | 1.89      | 0.07                  | 0.05 | 0.08 | 1.16                  | 1.25 | 0.23              | 0.44 |

# Germanium (Ge)



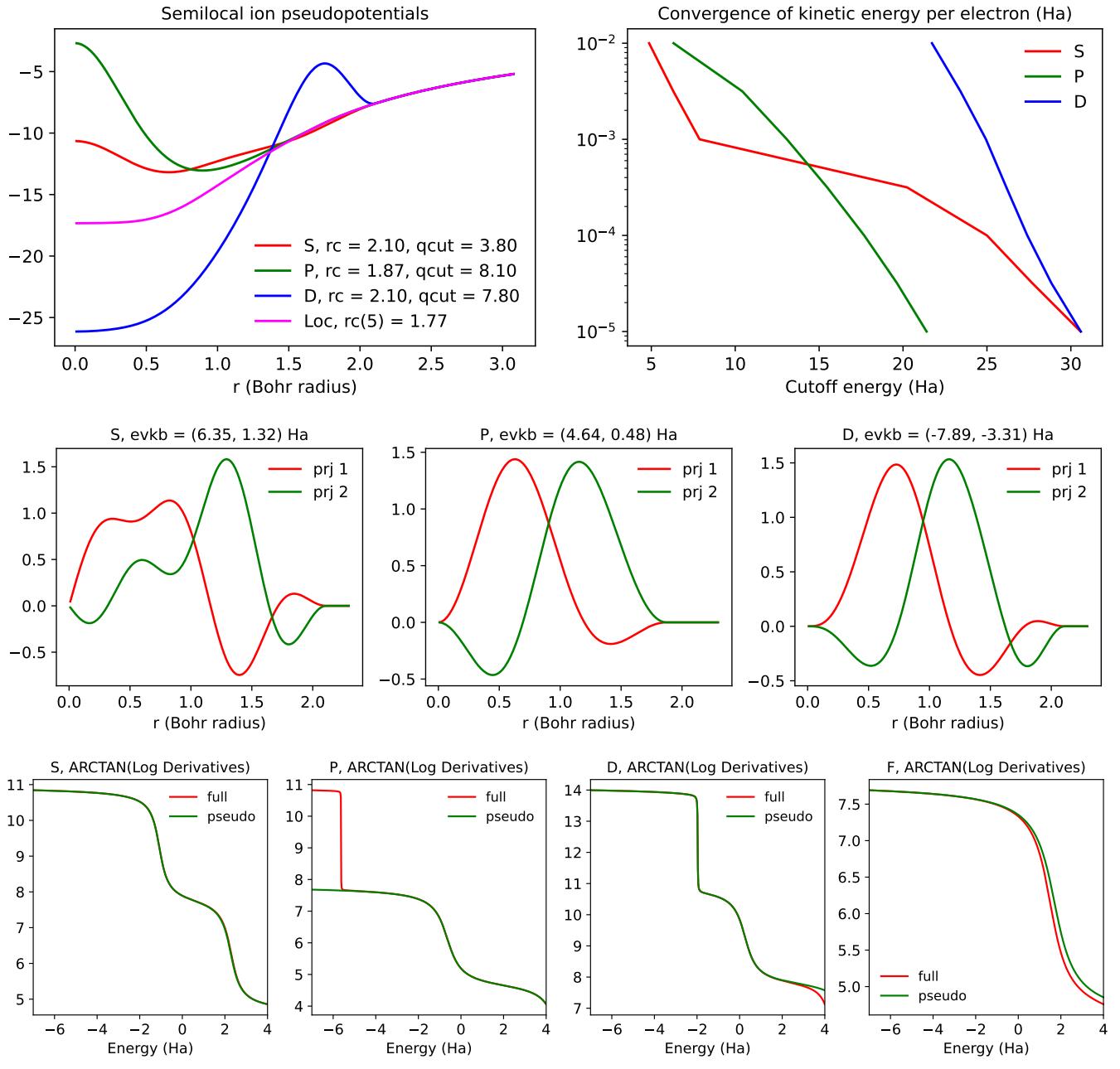
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 22                   | 25                   | 1.77                | 0.41     | 0.87      | 0.01                  | 0.05 | 0.17 | 1.21                  | 1.21 | 0.04              | 0.04 |
| PseudoDojo | 34                   | 37                   | 1.84                | 0.48     | 1.03      | 0.02                  | 0.05 | 0.08 | 1.50                  | 1.50 | 0.02              | 0.02 |
| SG15       | 19                   | 28                   | 2.81                | 1.03     | 2.20      | 0.11                  | 0.03 | 0.12 | 1.64                  | 1.64 | 0.01              | 0.01 |

# Arsenic (As)



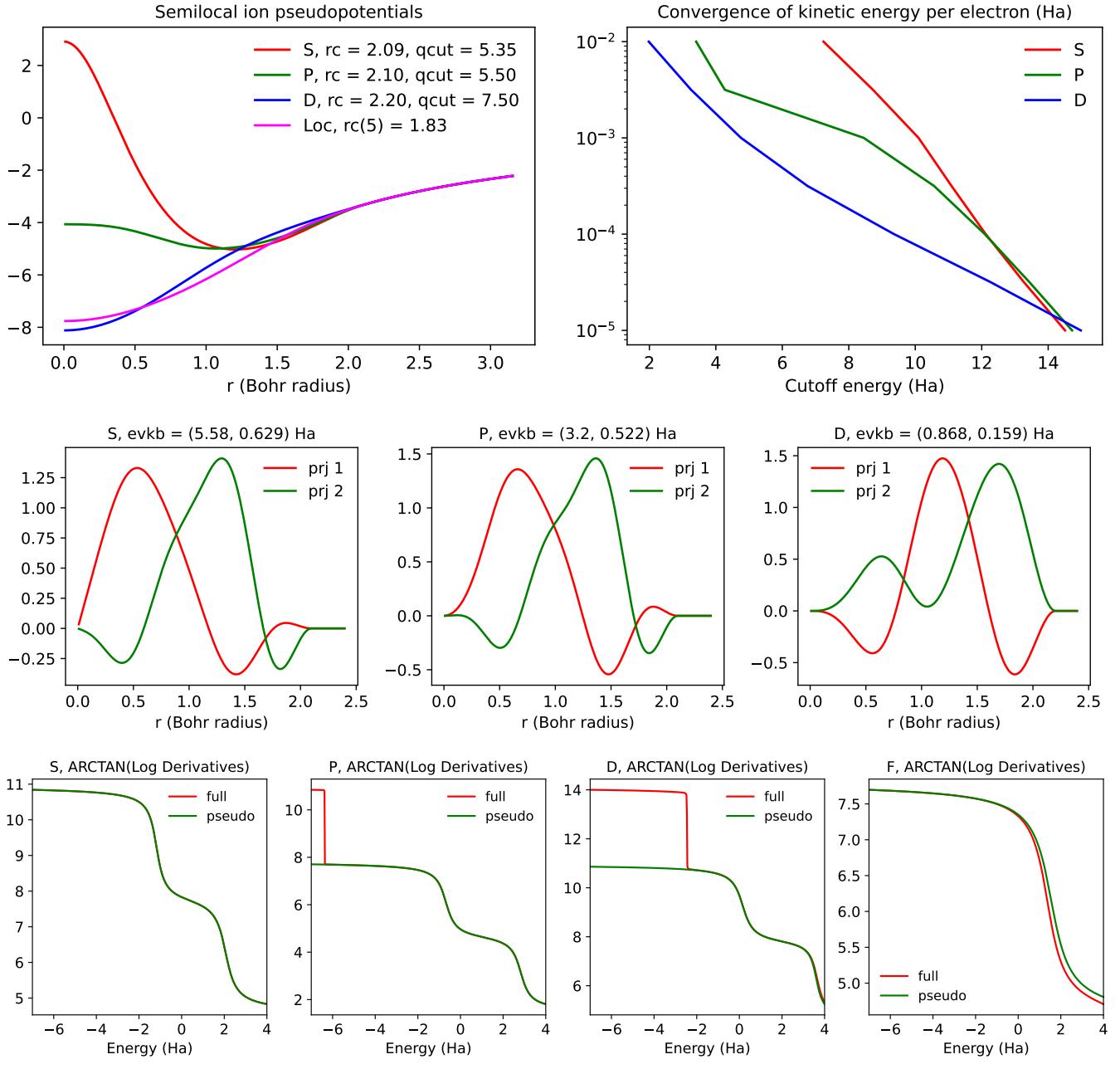
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 27                   | 30                   | 1.28                | 0.71     | 1.39      | 0.02                  | 0.05 | 0.05 | 0.19                  | 0.23 | 0.03              | 0.03 |
| PseudoDojo | 37                   | 40                   | 0.93                | 0.37     | 0.72      | 0.01                  | 0.00 | 0.05 | 0.18                  | 0.29 | 0.46              | 0.27 |
| SG15       | 12                   | 16                   | 0.90                | 1.19     | 2.31      | 0.01                  | 0.01 | 0.02 | 0.03                  | 0.04 | 0.21              | 0.05 |

# Selenium (Se)



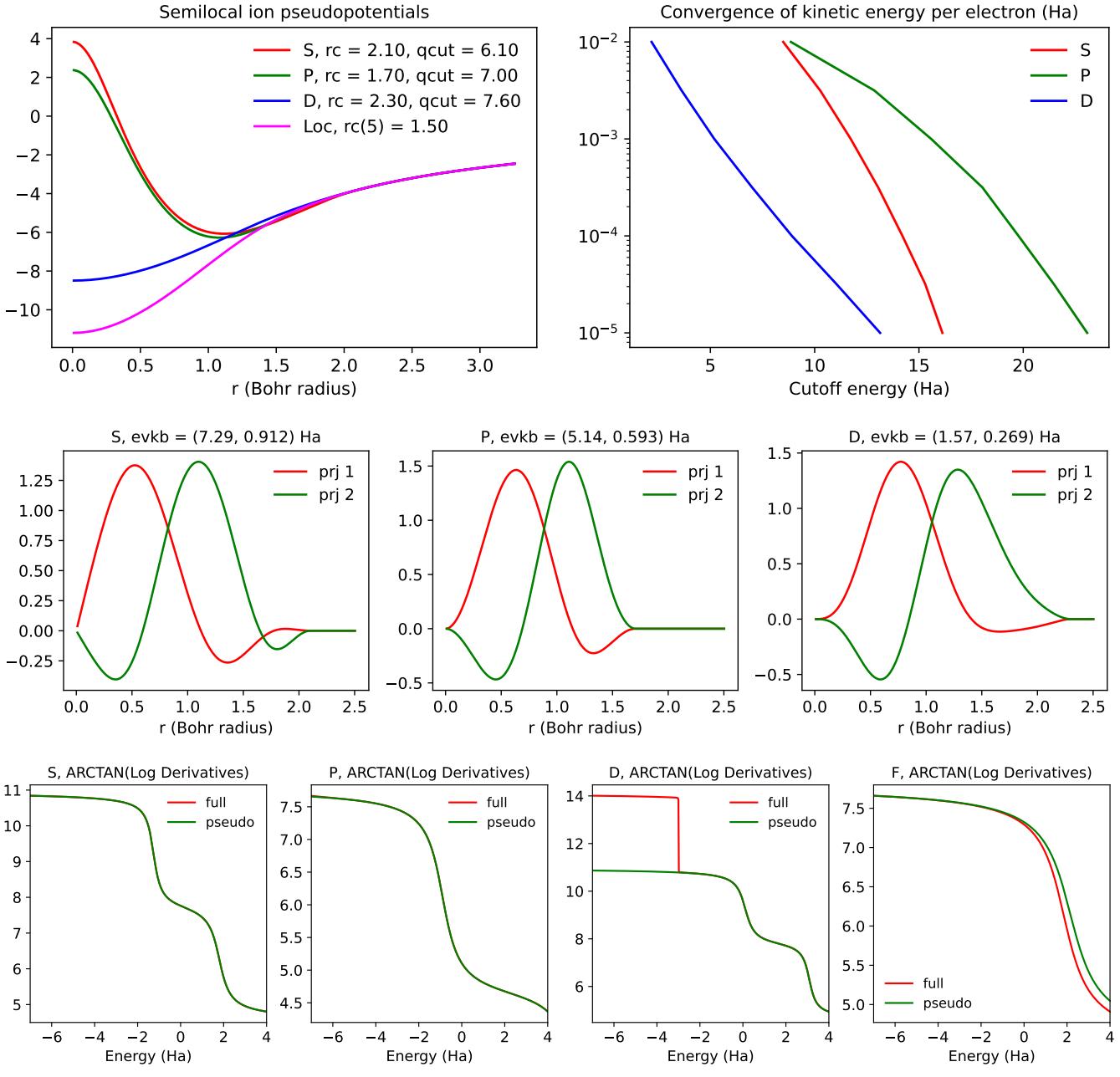
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 27                   | 30                   | 3.35                | 0.12     | 0.25      | 0.06                  | 0.10 | 0.14 | 0.36                  | 0.36 | 0.15              | 0.08 |
| PseudoDojo | 37                   | 40                   | 3.81                | 0.24     | 0.51      | 0.06                  | 0.09 | 0.13 | 0.10                  | 0.10 | 0.46              | 0.15 |
| SG15       | 12                   | 15                   | 5.23                | 0.64     | 1.36      | 0.04                  | 0.07 | 0.09 | 0.23                  | 0.24 | 0.00              | 0.03 |

# Bromine (Br)



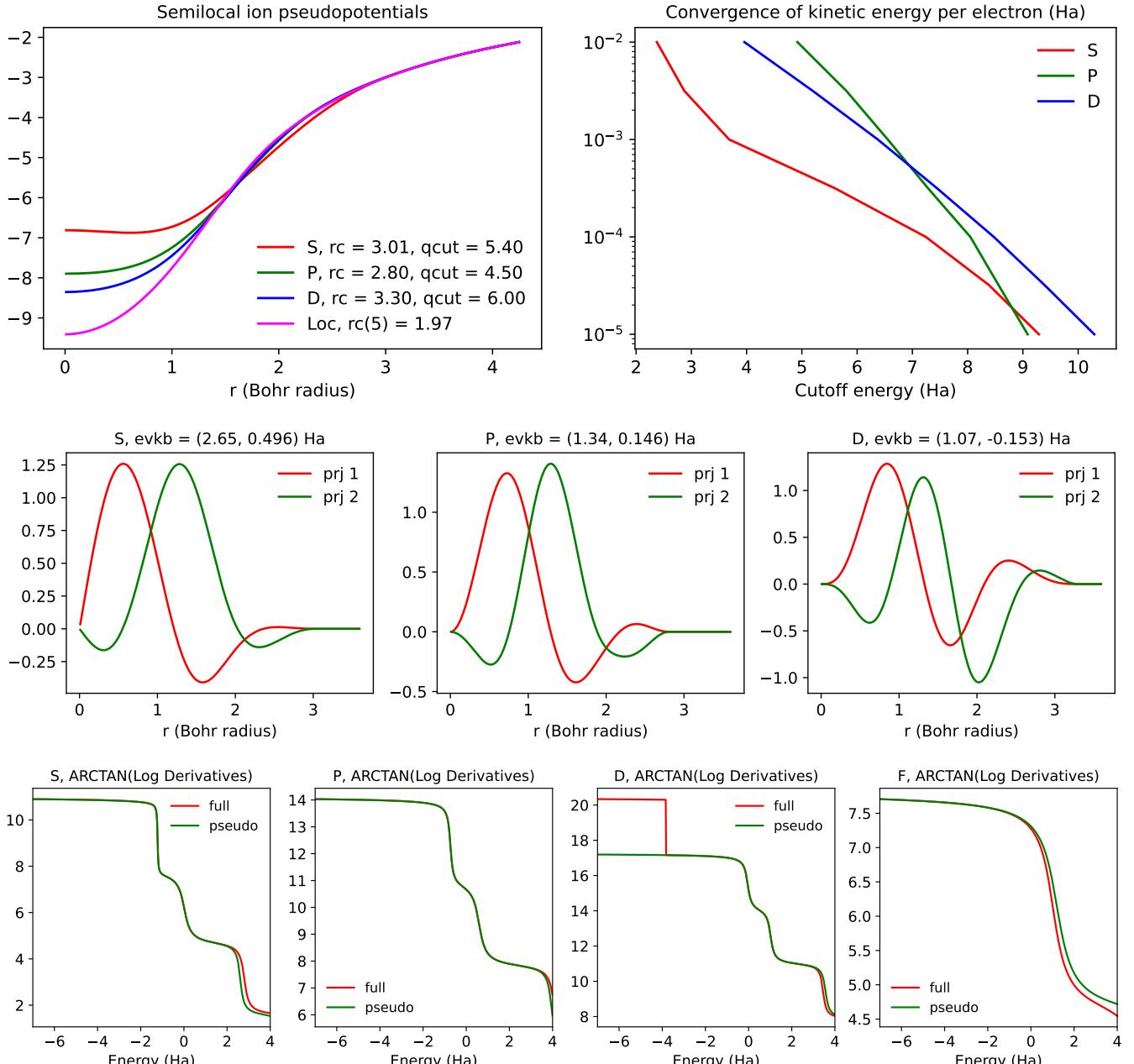
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 11                   | 14                   | 1.09                | 0.15     | 0.49      | 0.06                  | 0.01 | 0.22 | 0.21                  | 0.17 | 0.05              | 0.11 |
| PseudoDojo | 16                   | 20                   | 1.27                | 0.05     | 0.17      | 0.05                  | 0.01 | 0.17 | 0.19                  | 0.21 | 2.77              | 0.42 |
| SG15       | 10                   | 25                   | 0.62                | 1.10     | 3.72      | 0.08                  | 0.03 | 0.18 | 0.22                  | 0.88 | 0.47              | 0.03 |

# Krypton (Kr)



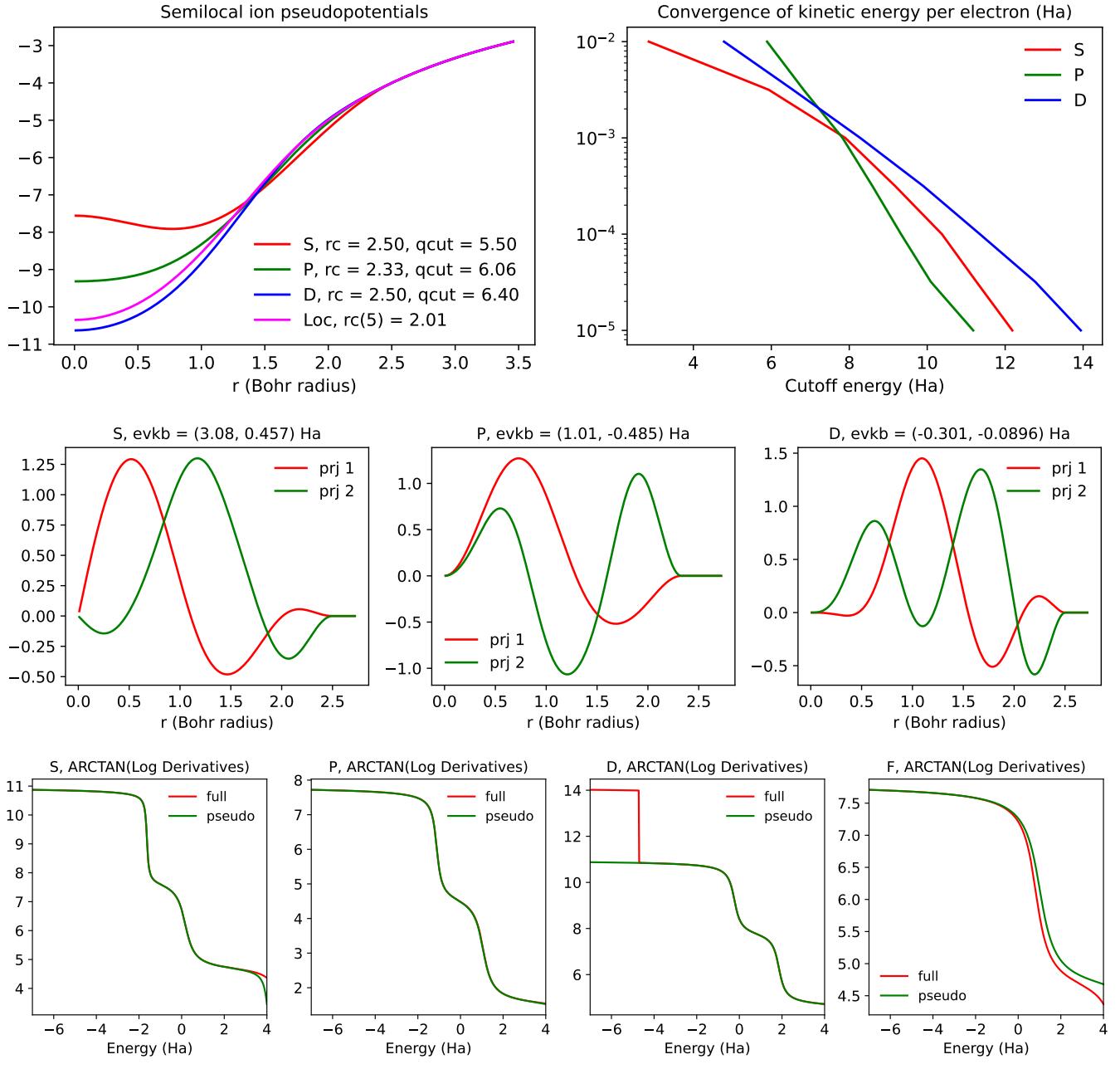
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |     |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |       |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|-----|------|-----------------------|------|-------------------|-------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC | COMP | LAP                   | HAP  | LOP               | HOP   |
| SPMS       | 19                   | 22                   | 7.04                | 0.03     | 2.27      | -                     | -   | -    | 0.06                  | 0.06 | 0.82              | 1.02  |
| PseudoDojo | 19                   | 23                   | 7.04                | 0.03     | 2.29      | -                     | -   | -    | 0.08                  | 0.08 | 1.65              | 1.44  |
| SG15       | 8                    | 10                   | 7.17                | 0.04     | 2.62      | -                     | -   | -    | 0.07                  | 0.07 | 20.64             | 18.18 |

# Rubidium (Rb)



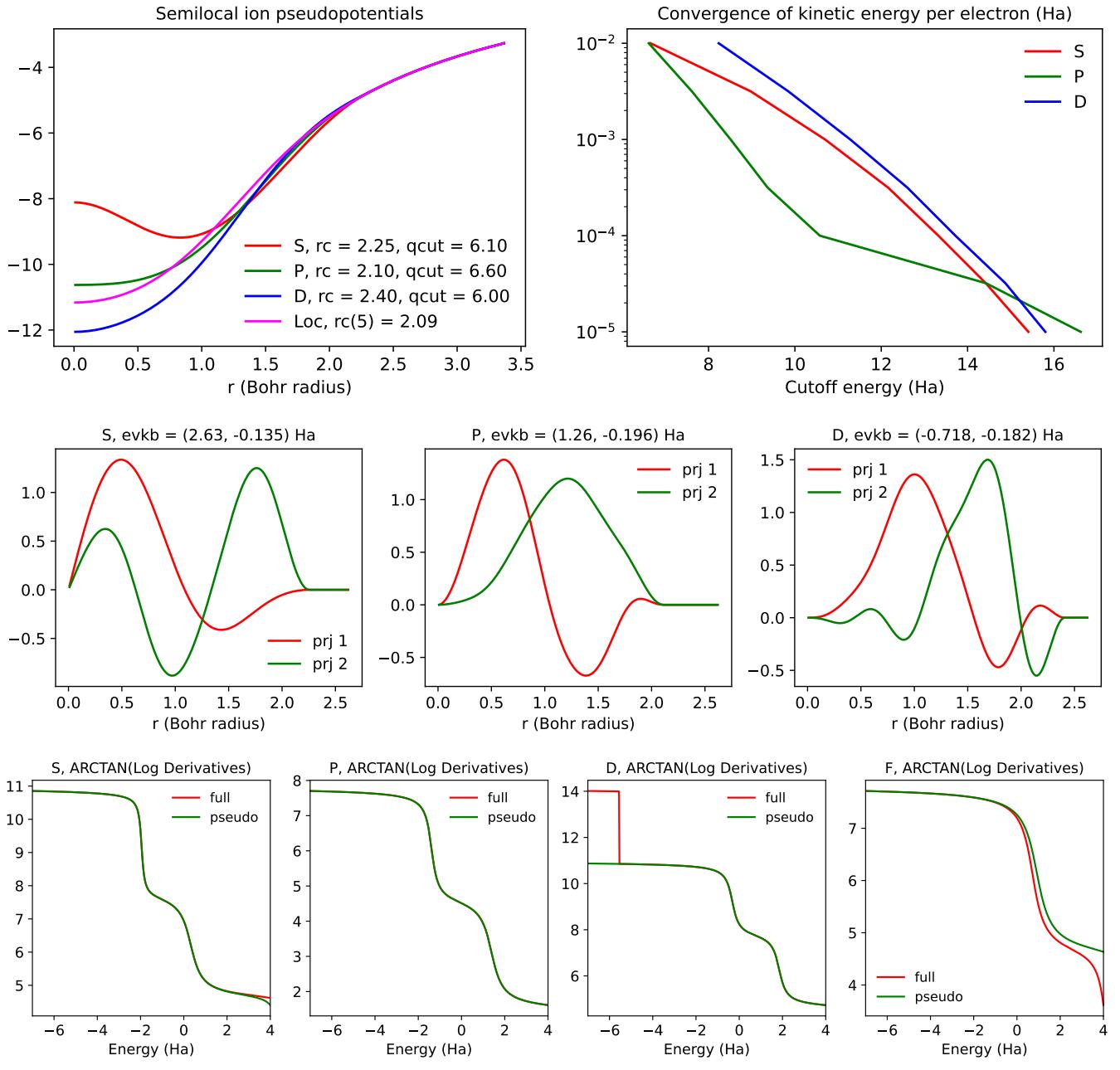
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 7                    | 9                    | 0.38                | 0.24     | 2.90      | 0.06                  | 0.05 | 0.09 | 0.02                  | 0.02 | 0.25              | 0.25 |
| PseudoDojo | 18                   | 23                   | 0.38                | 0.24     | 2.88      | 0.06                  | 0.06 | 0.10 | 0.10                  | 0.10 | 0.02              | 0.02 |
| SG15       | 8                    | 9                    | 0.39                | 0.24     | 2.85      | 0.06                  | 0.06 | 0.09 | 0.02                  | 0.02 | 0.42              | 0.42 |

# Strontium (Sr)



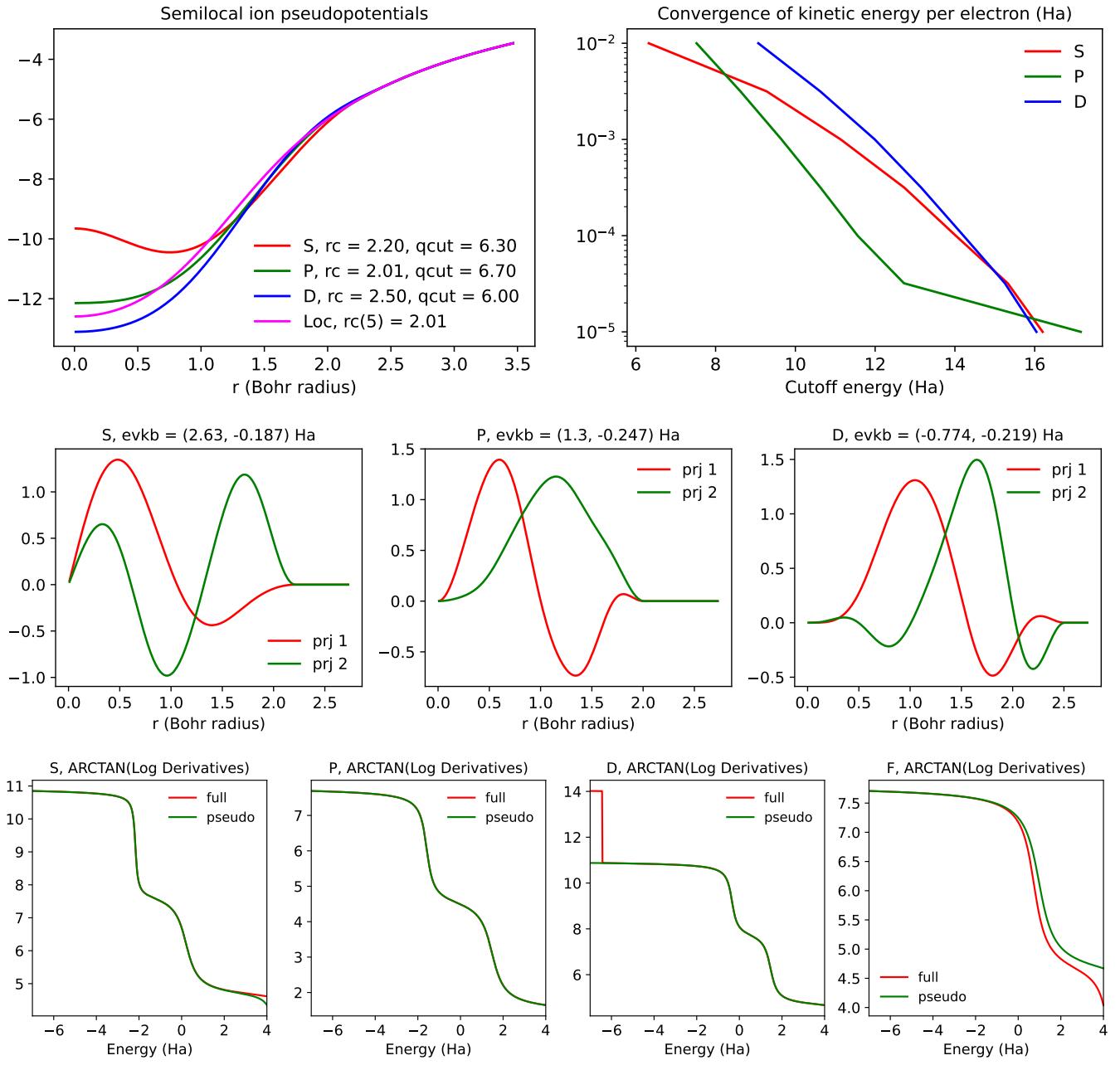
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 10                   | 13                   | 0.92                | 0.97     | 4.48      | 0.06                  | 0.09 | 0.19 | 0.20                  | 0.20 | 0.02              | 0.06 |
| PseudoDojo | 26                   | 31                   | 1.17                | 1.32     | 6.10      | 0.15                  | 0.17 | 0.19 | 0.19                  | 0.19 | 0.01              | 0.00 |
| SG15       | 9                    | 12                   | 1.02                | 1.21     | 5.58      | 0.12                  | 0.15 | 0.14 | 0.13                  | 0.13 | 0.07              | 0.13 |

# Yttrium (Y)



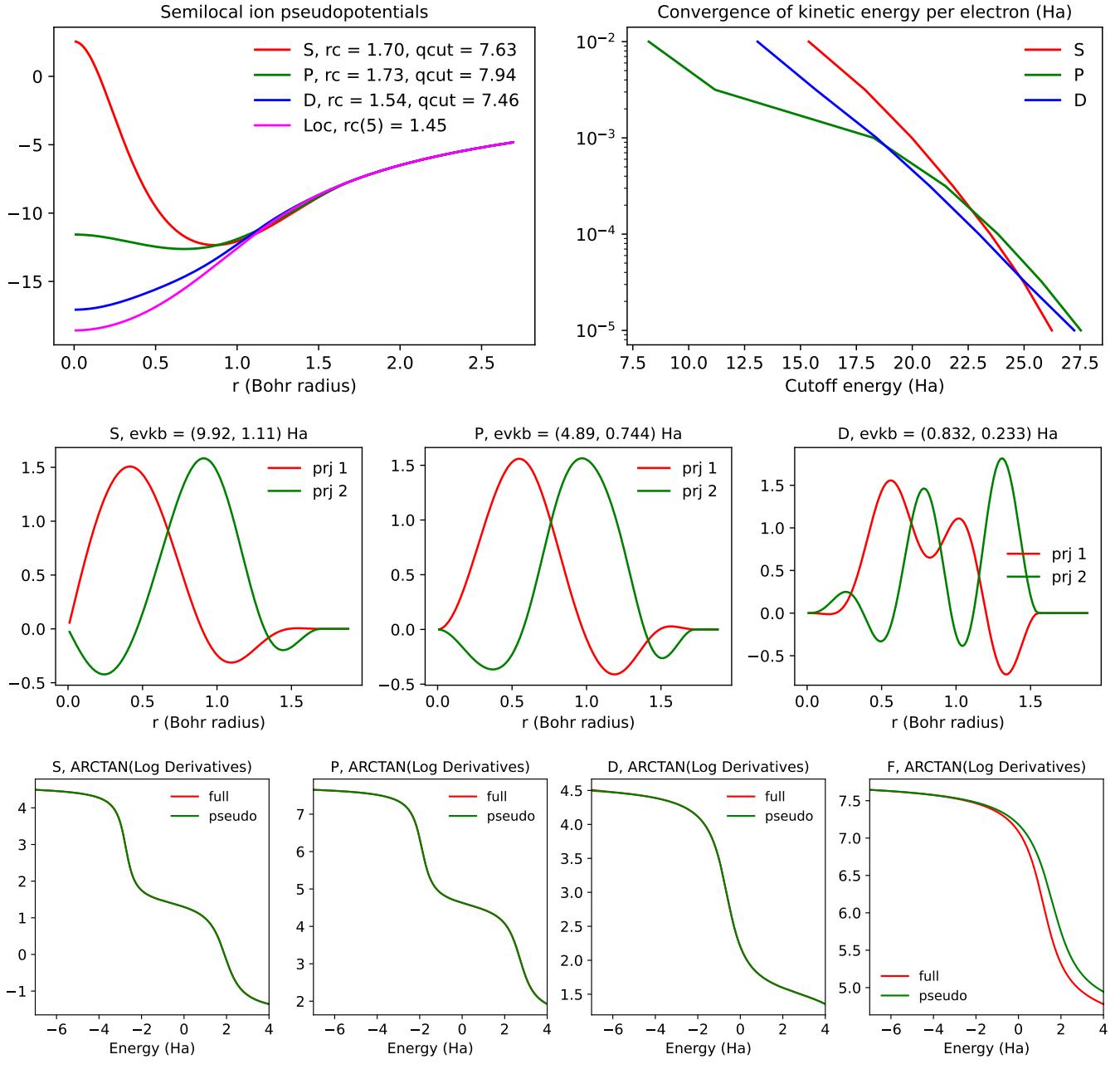
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 13                   | 16                   | 2.67                | 1.09     | 2.46      | 0.15                  | 0.16 | 0.06 | 0.38                  | 0.31 | 0.00              | 0.05 |
| PseudoDojo | 28                   | 33                   | 2.74                | 1.00     | 2.26      | 0.16                  | 0.17 | 0.06 | 0.46                  | 0.33 | 0.02              | 0.02 |
| SG15       | 17                   | 26                   | 2.85                | 0.96     | 2.16      | 0.17                  | 0.17 | 0.04 | 0.18                  | 0.37 | 0.01              | 0.01 |

# Zirconium (Zr)



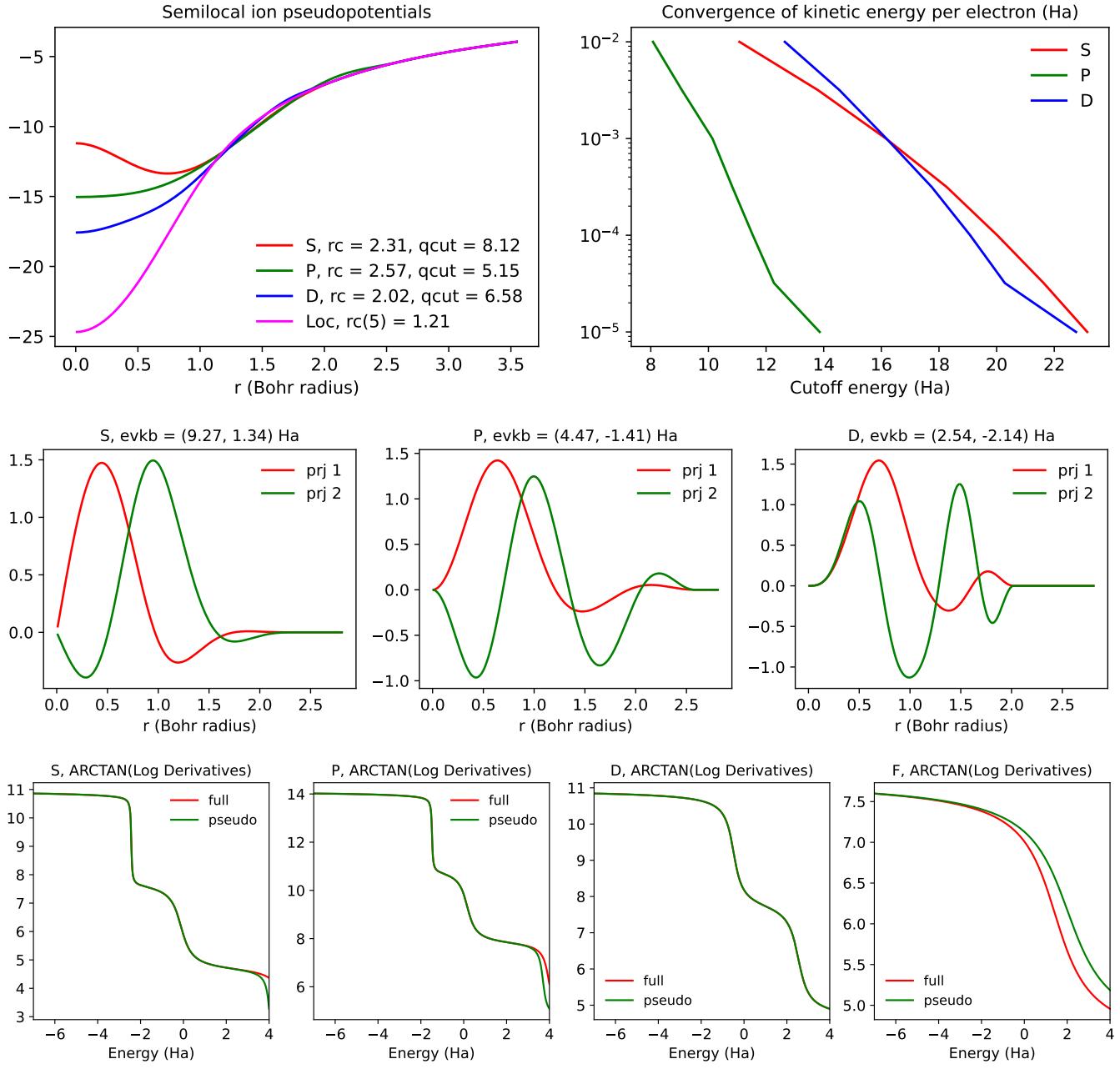
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |     |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|-----|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP |
| SPMS       | 13                   | 17                   | 2.35                | 1.33     | 1.82      | 0.01                  | 0.03 | 0.07 | 0.97                  | 0.70 | 0.12              | 0.0 |
| PseudoDojo | 26                   | 31                   | 1.51                | 0.77     | 1.06      | 0.02                  | 0.01 | 0.09 | 1.03                  | 0.76 | 0.06              | 0.0 |
| SG15       | 22                   | 29                   | 2.58                | 0.52     | 0.72      | 0.04                  | 0.03 | 0.07 | 0.29                  | 0.35 | 0.02              | 0.0 |

# Niobium (Nb)



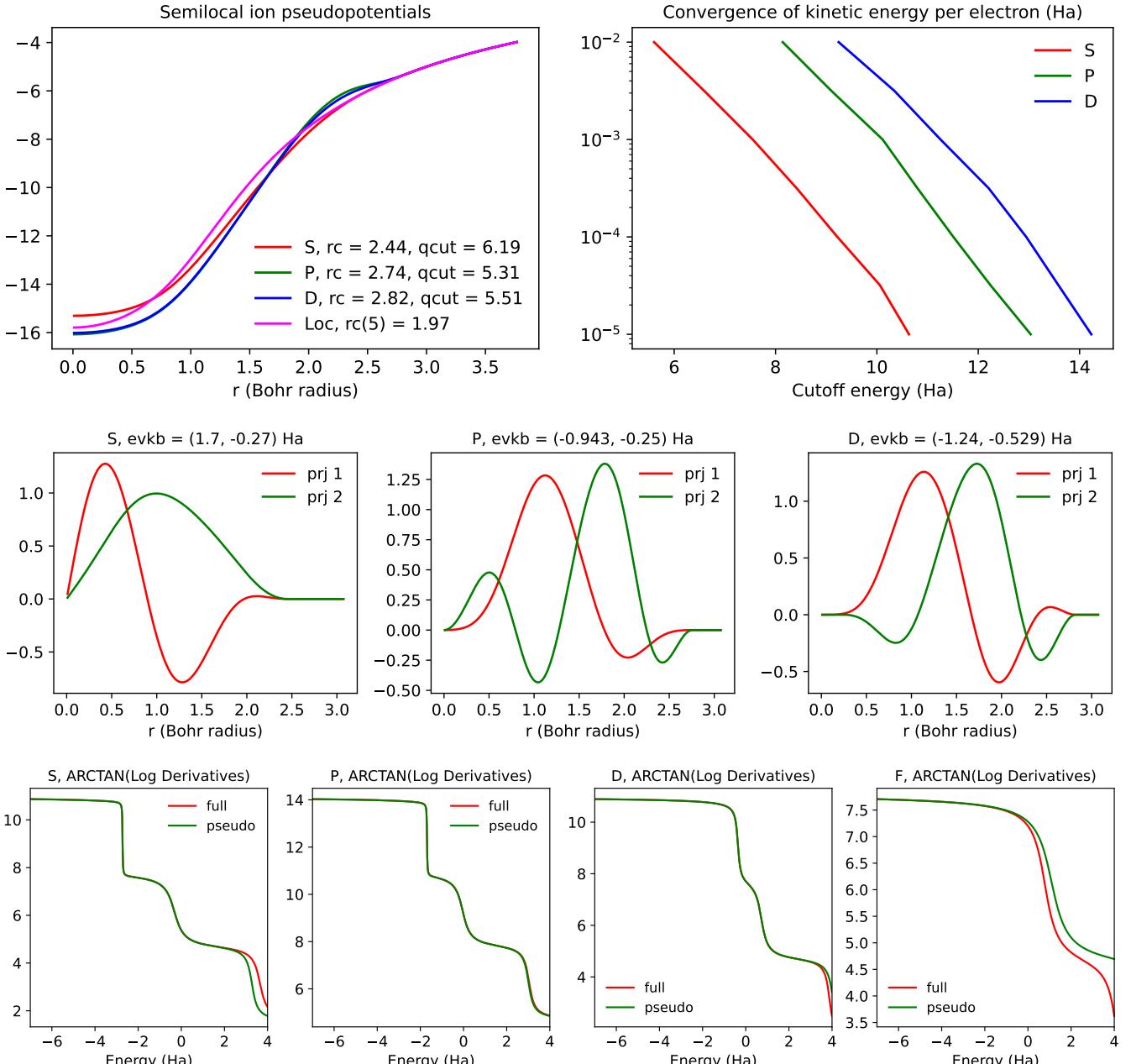
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 24                   | 28                   | 1.18                | 1.53     | 1.50      | 0.03                  | 0.02 | 0.10 | 0.88                  | 0.88 | 0.01              | 0.01 |
| PseudoDojo | 33                   | 39                   | 1.04                | 1.29     | 1.26      | 0.01                  | 0.01 | 0.10 | 0.69                  | 0.69 | 0.00              | 0.00 |
| SG15       | 41                   | 72                   | 1.42                | 1.35     | 1.32      | 0.02                  | 0.01 | 0.09 | 1.40                  | 1.40 | 0.00              | 0.00 |

# Molybdenum (Mo)



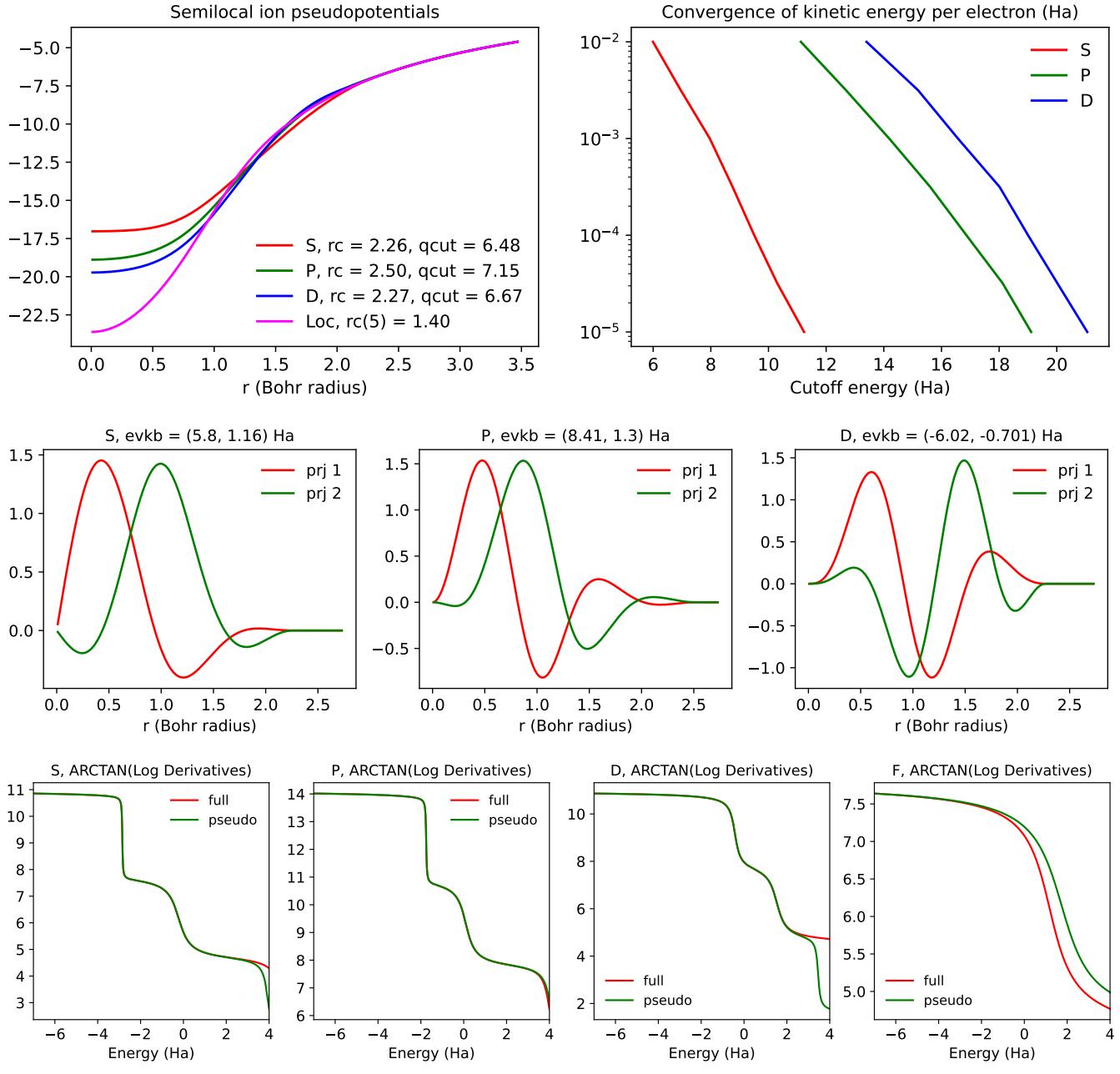
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 19                   | 23                   | 1.30                | 1.60     | 1.17      | 0.08                  | 0.03 | 0.13 | 0.25                  | 0.25 | 0.01              | 0.01 |
| PseudoDojo | 32                   | 38                   | 1.24                | 1.41     | 1.03      | 0.09                  | 0.02 | 0.12 | 0.47                  | 0.47 | 0.12              | 0.12 |
| SG15       | 15                   | 19                   | 4.20                | 0.12     | 0.09      | 0.14                  | 0.03 | 0.13 | 0.30                  | 0.30 | 0.07              | 0.07 |

# Technetium (Tc)



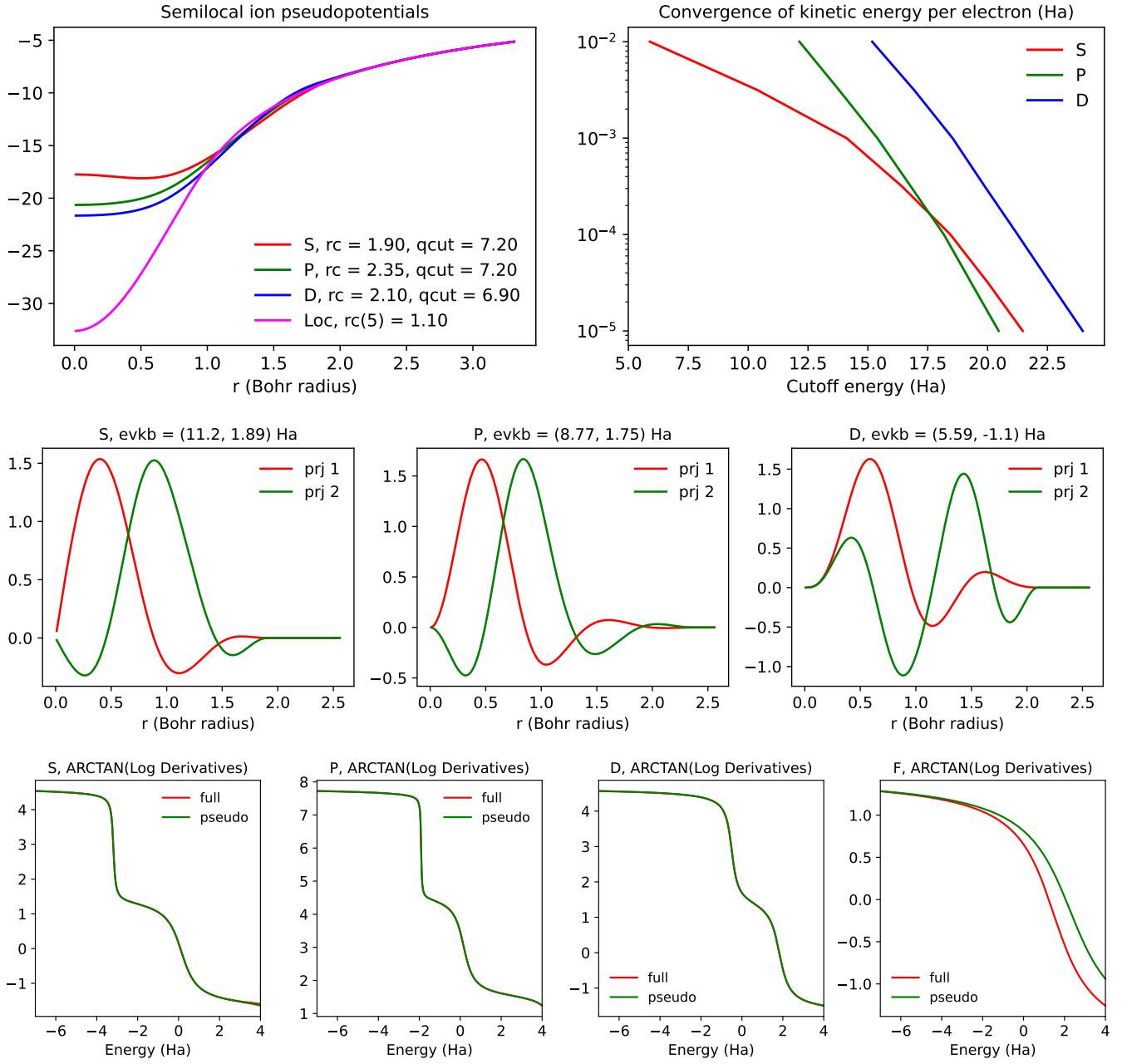
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 12                   | 14                   | 4.32                | 0.61     | 0.43      | 0.02                  | 0.08 | 0.11 | 3.21                  | 2.27 | 0.50              | 0.07 |
| PseudoDojo | 34                   | 39                   | 0.94                | 1.63     | 1.14      | 0.01                  | 0.11 | 0.13 | 3.91                  | 2.75 | 0.10              | 0.02 |
| SG15       | 15                   | 26                   | 2.99                | 0.75     | 0.52      | 0.03                  | 0.08 | 0.10 | 0.17                  | 0.08 | 0.31              | 0.05 |

# Ruthenium (Ru)



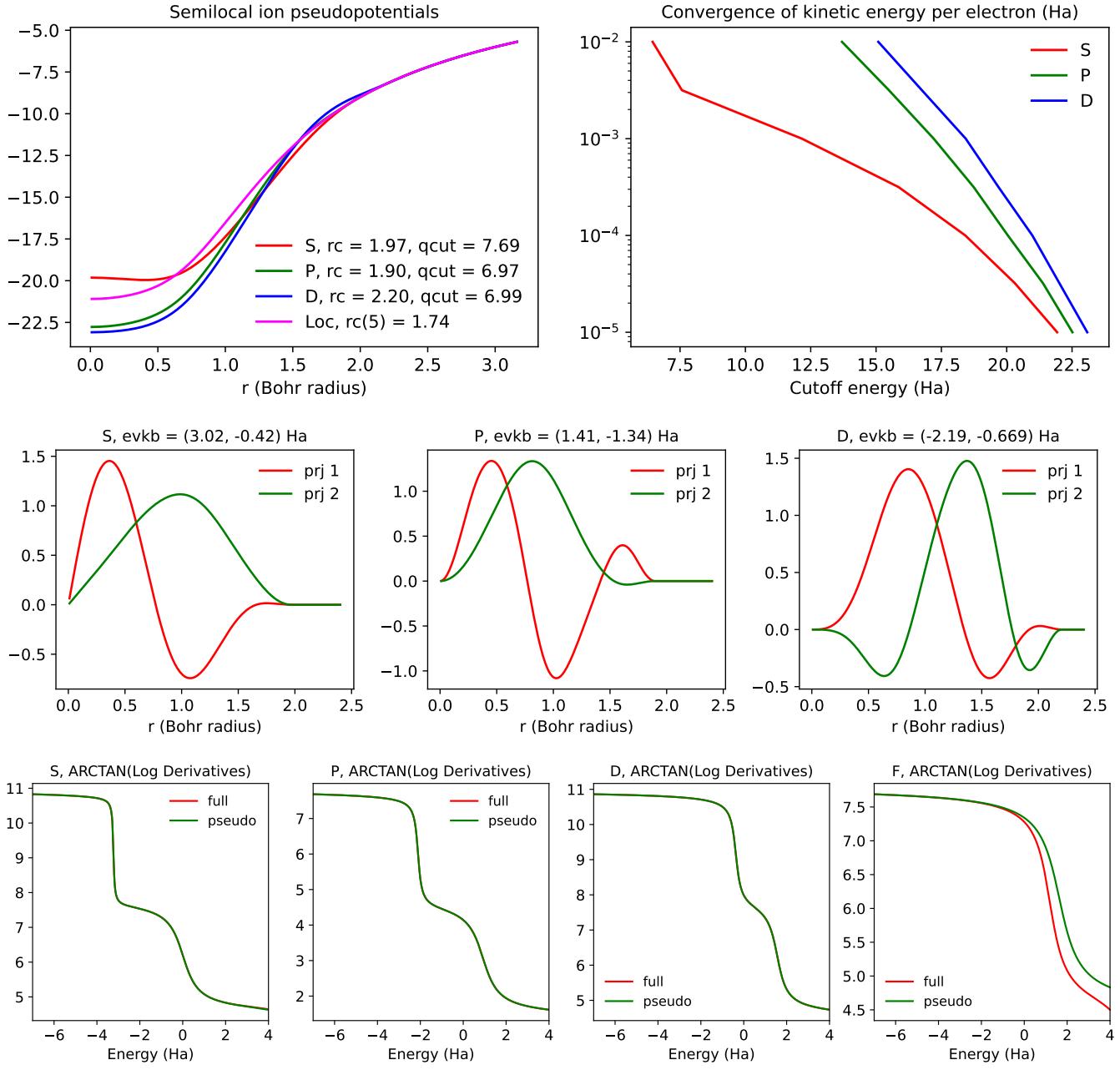
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 19                   | 24                   | 2.81                | 2.35     | 1.63      | 0.19                  | 0.16 | 0.12 | 5.38                  | 3.80 | 0.01              | 0.02 |
| PseudoDojo | 35                   | 42                   | 2.82                | 2.12     | 1.48      | 0.19                  | 0.15 | 0.12 | 5.79                  | 4.10 | 0.01              | 0.00 |
| SG15       | 17                   | 27                   | 2.20                | 1.12     | 0.78      | 0.15                  | 0.12 | 0.08 | 0.03                  | 0.18 | 0.02              | 0.05 |

# Rhodium (Rh)



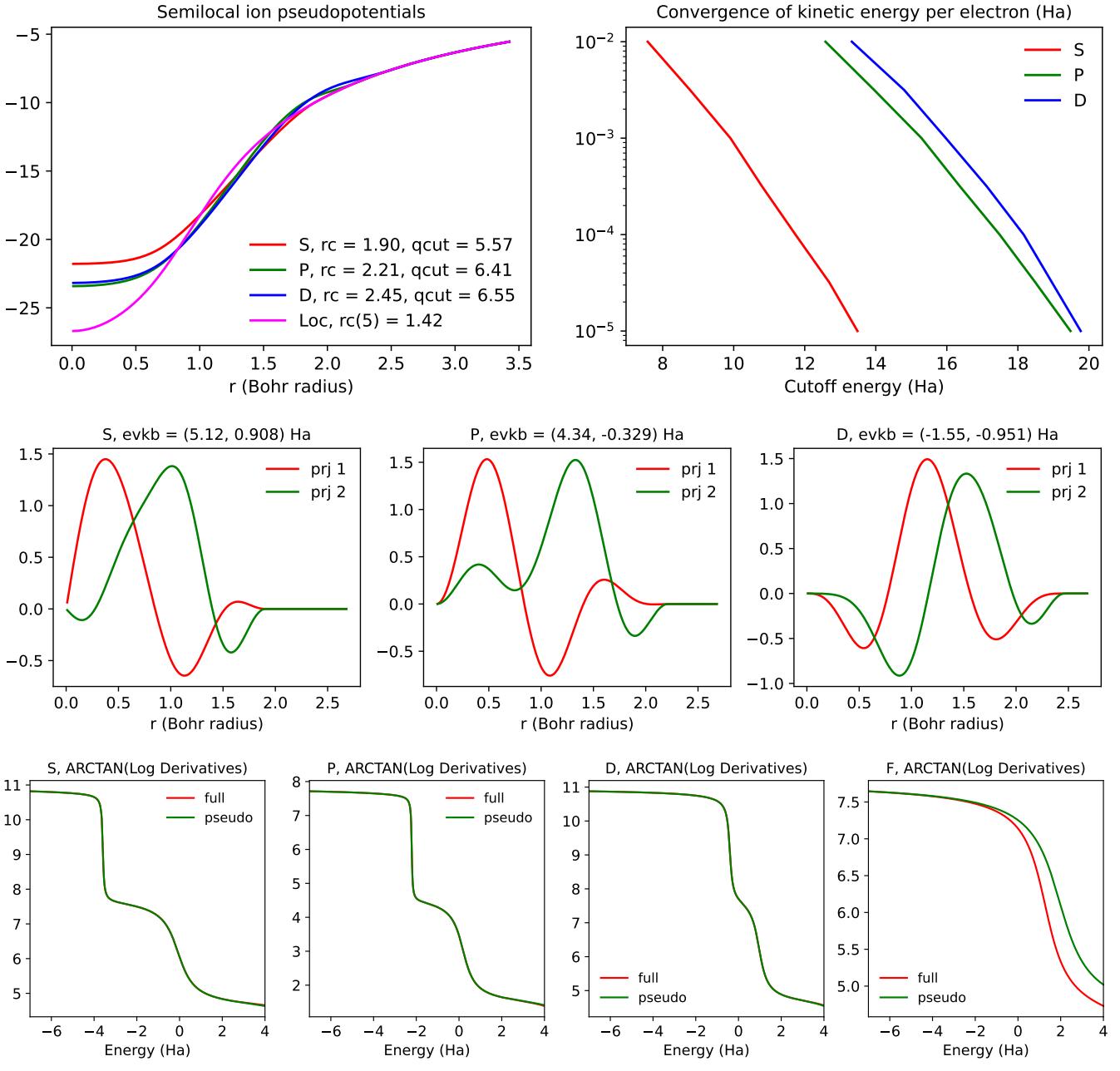
|            | $E_{cut}$            |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{lat}$ |      |      | $\delta_{asr}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|----------------|------|------|----------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC            | FCC  | COMP | LAP            | HAP  | LOP               | HOP  |
| SPMS       | 21                   | 25                   | 1.53                | 2.61     | 2.17      | 0.13           | 0.11 | 0.09 | 0.08           | 0.08 | 0.02              | 0.01 |
| PseudoDojo | 37                   | 42                   | 1.36                | 2.56     | 2.14      | 0.14           | 0.11 | 0.09 | 0.93           | 0.93 | 0.05              | 0.04 |
| SG15       | 20                   | 33                   | 2.55                | 2.02     | 1.69      | 0.10           | 0.09 | 0.06 | 0.46           | 0.46 | 0.11              | 0.13 |

# Palladium (Pd)



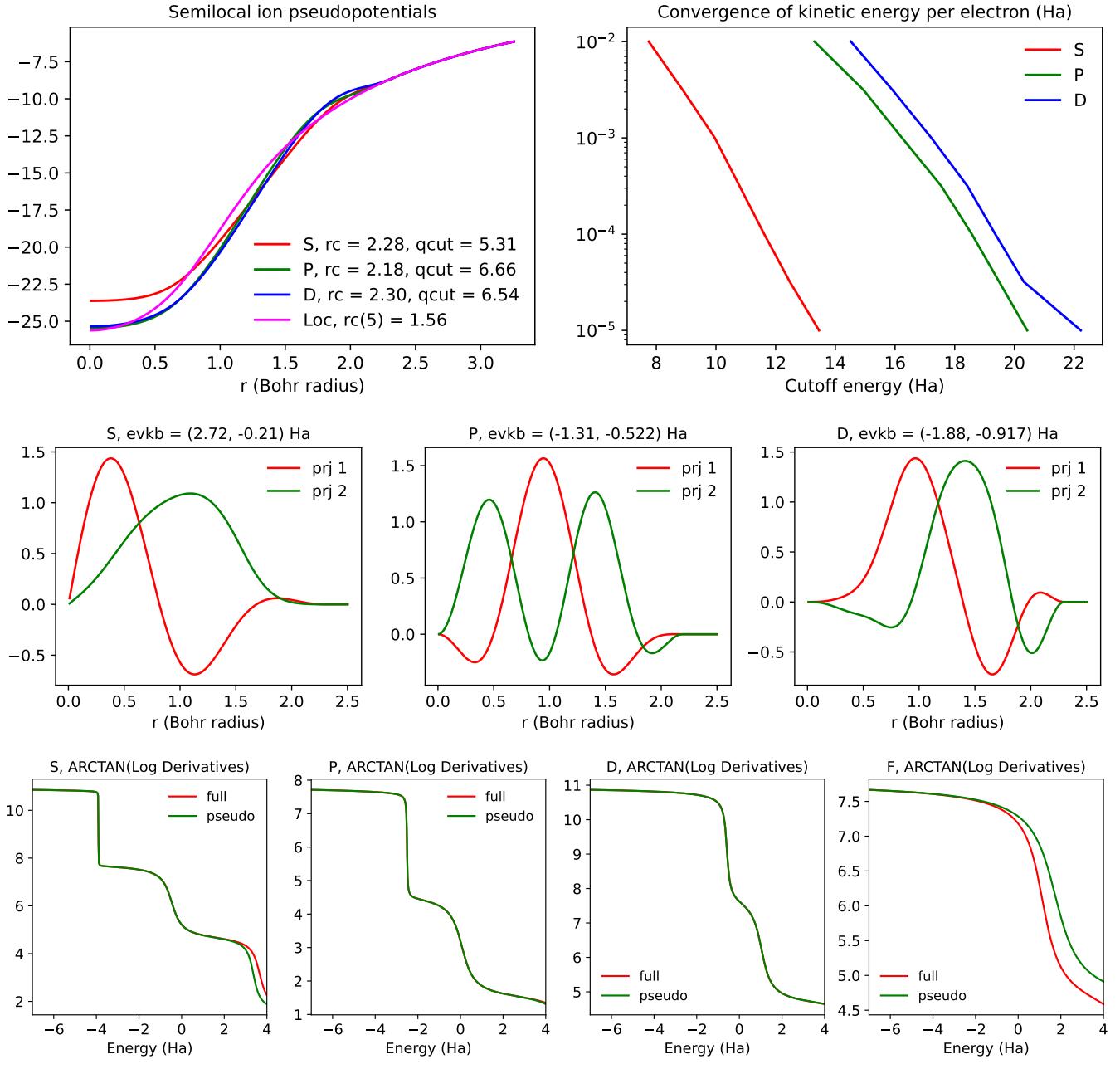
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 21                   | 24                   | 1.95                | 3.70     | 4.27      | 0.11                  | 0.09 | 0.10 | 0.38                  | 0.38 | 0.02              | 0.03 |
| PseudoDojo | 34                   | 39                   | 3.95                | 1.14     | 1.32      | 0.05                  | 0.06 | 0.11 | 0.11                  | 0.11 | 0.01              | 0.02 |
| SG15       | 23                   | 41                   | 2.51                | 1.60     | 1.87      | 0.02                  | 0.03 | 0.10 | 0.09                  | 0.09 | 0.04              | 0.02 |

# Silver (Ag)



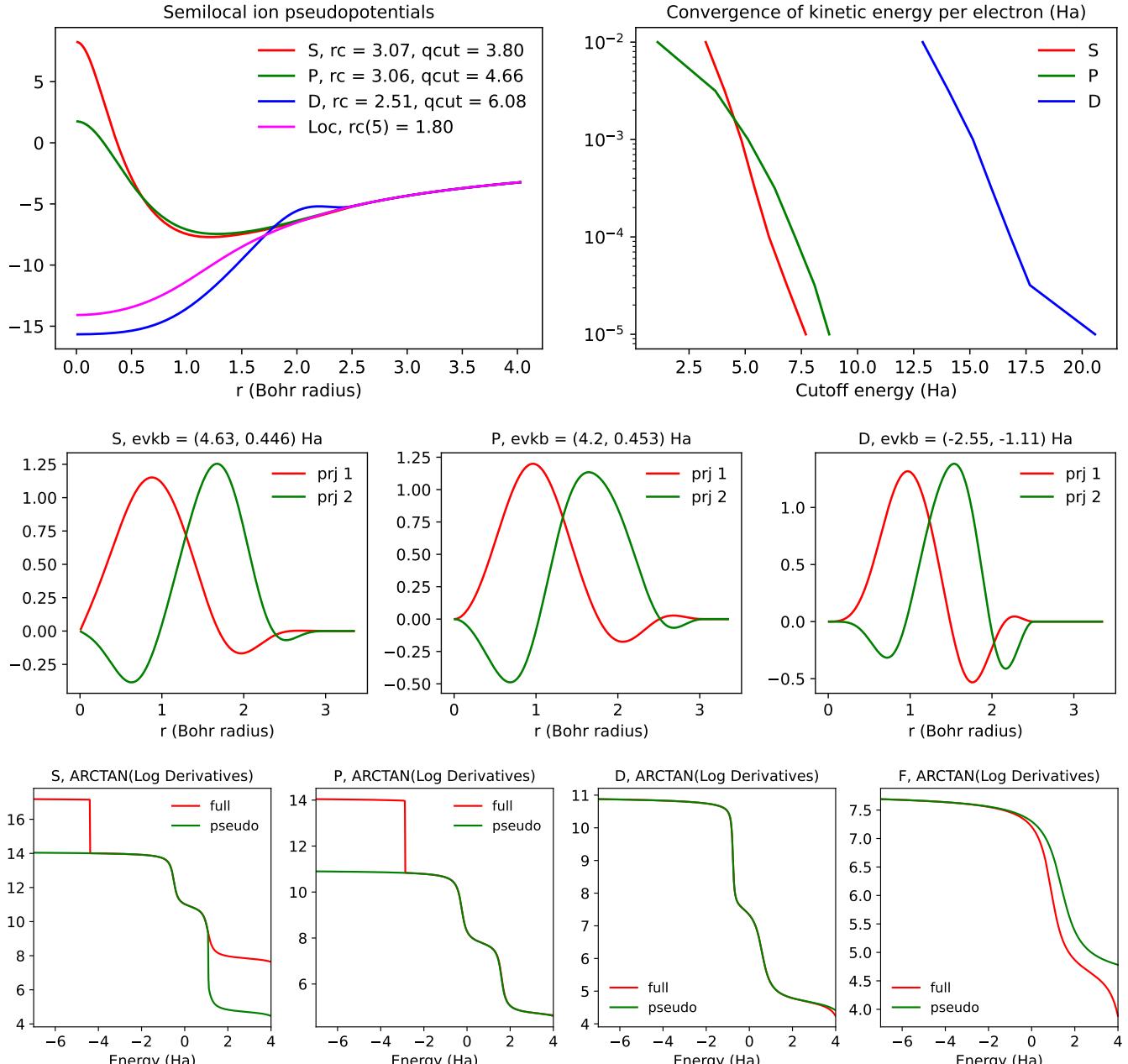
|            | $E_{cut}$            |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{lat}$ |      |      | $\delta_{asr}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|----------------|------|------|----------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC            | FCC  | COMP | LAP            | HAP  | LOP               | HOP  |
| SPMS       | 18                   | 22                   | 1.14                | 0.29     | 0.52      | 0.09           | 0.14 | 0.13 | 0.42           | 0.42 | 0.03              | 0.03 |
| PseudoDojo | 36                   | 40                   | 0.96                | 0.32     | 0.58      | 0.13           | 0.17 | 0.11 | 0.59           | 0.59 | 0.00              | 0.00 |
| SG15       | 22                   | 24                   | 1.12                | 0.35     | 0.65      | 0.14           | 0.17 | 0.11 | 0.28           | 0.28 | 0.13              | 0.15 |

# Cadmium (Cd)



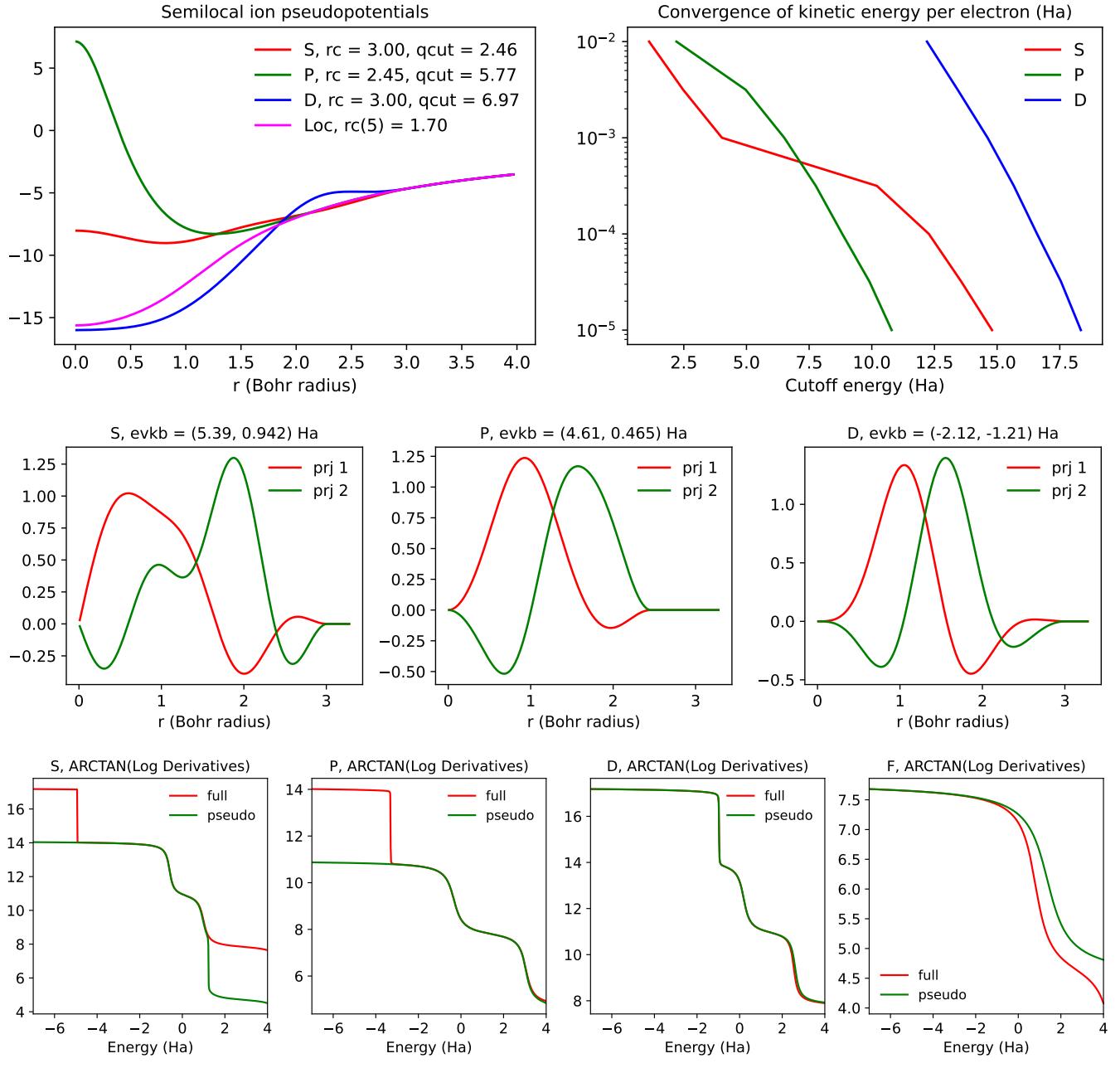
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |       | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|-------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP   | LOP               | HOP  |
| SPMS       | 19                   | 24                   | 0.40                | 0.43     | 1.28      | 0.01                  | 0.05 | 0.06 | 14.72                 | 10.41 | 0.16              | 0.11 |
| PseudoDojo | 44                   | 49                   | 1.26                | 1.13     | 3.45      | 0.11                  | 0.07 | 0.06 | 22.51                 | 15.92 | 0.06              | 0.11 |
| SG15       | 16                   | 18                   | 1.47                | 1.65     | 5.00      | 0.15                  | 0.13 | 0.07 | 0.19                  | 0.16  | 0.65              | 0.31 |

# Indium (In)



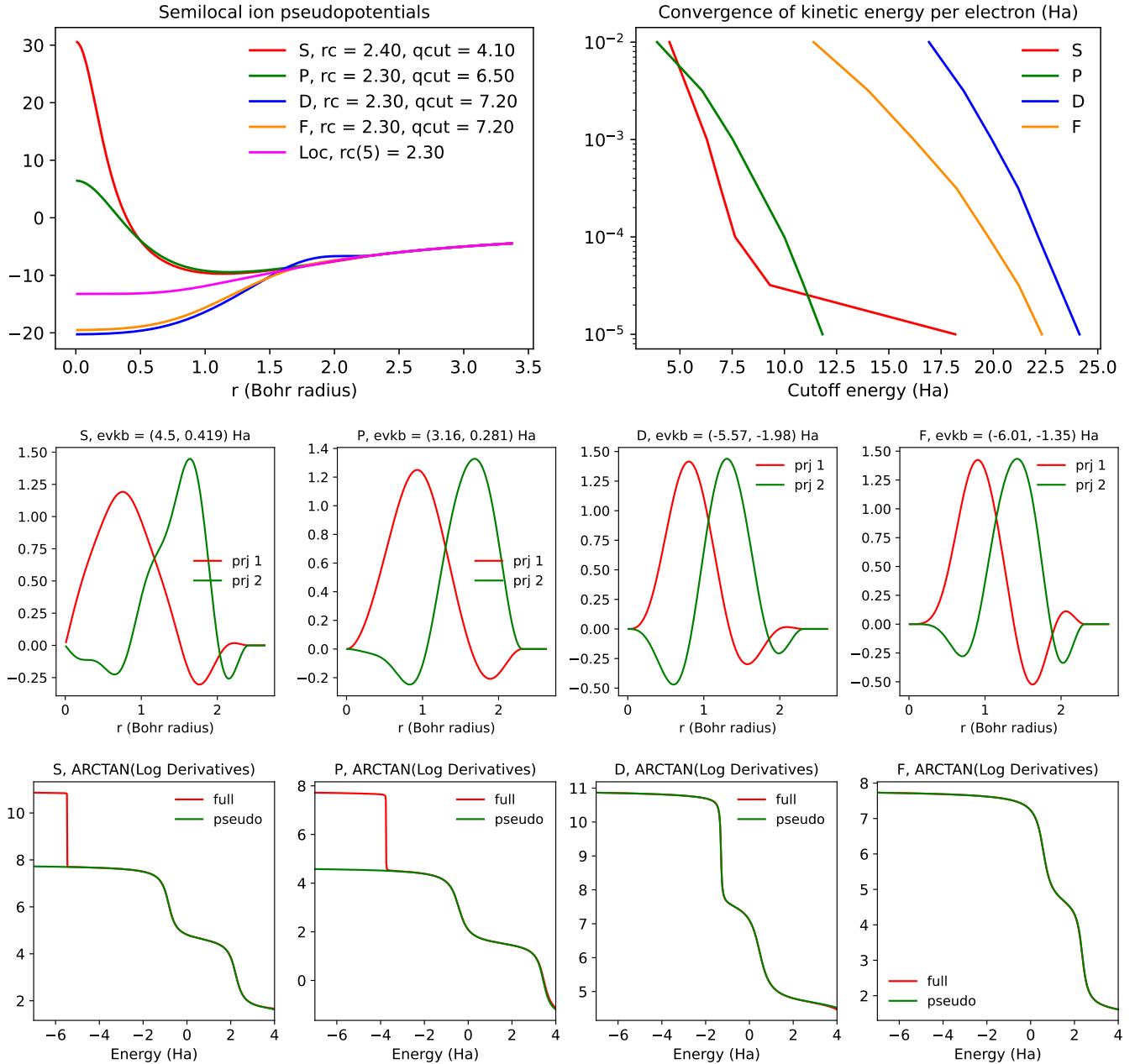
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 17                   | 20                   | 0.40                | 0.39     | 1.22      | 0.05                  | 0.03 | 0.10 | 0.44                  | 0.31 | 0.03              | 0.01 |
| PseudoDojo | 30                   | 33                   | 0.88                | 0.07     | 0.21      | 0.02                  | 0.04 | 0.05 | 0.30                  | 0.45 | 0.08              | 0.00 |
| SG15       | 26                   | 33                   | 0.40                | 0.40     | 1.25      | 0.05                  | 0.03 | 0.09 | 0.24                  | 0.18 | 0.02              | 0.01 |

# Tin (Sn)



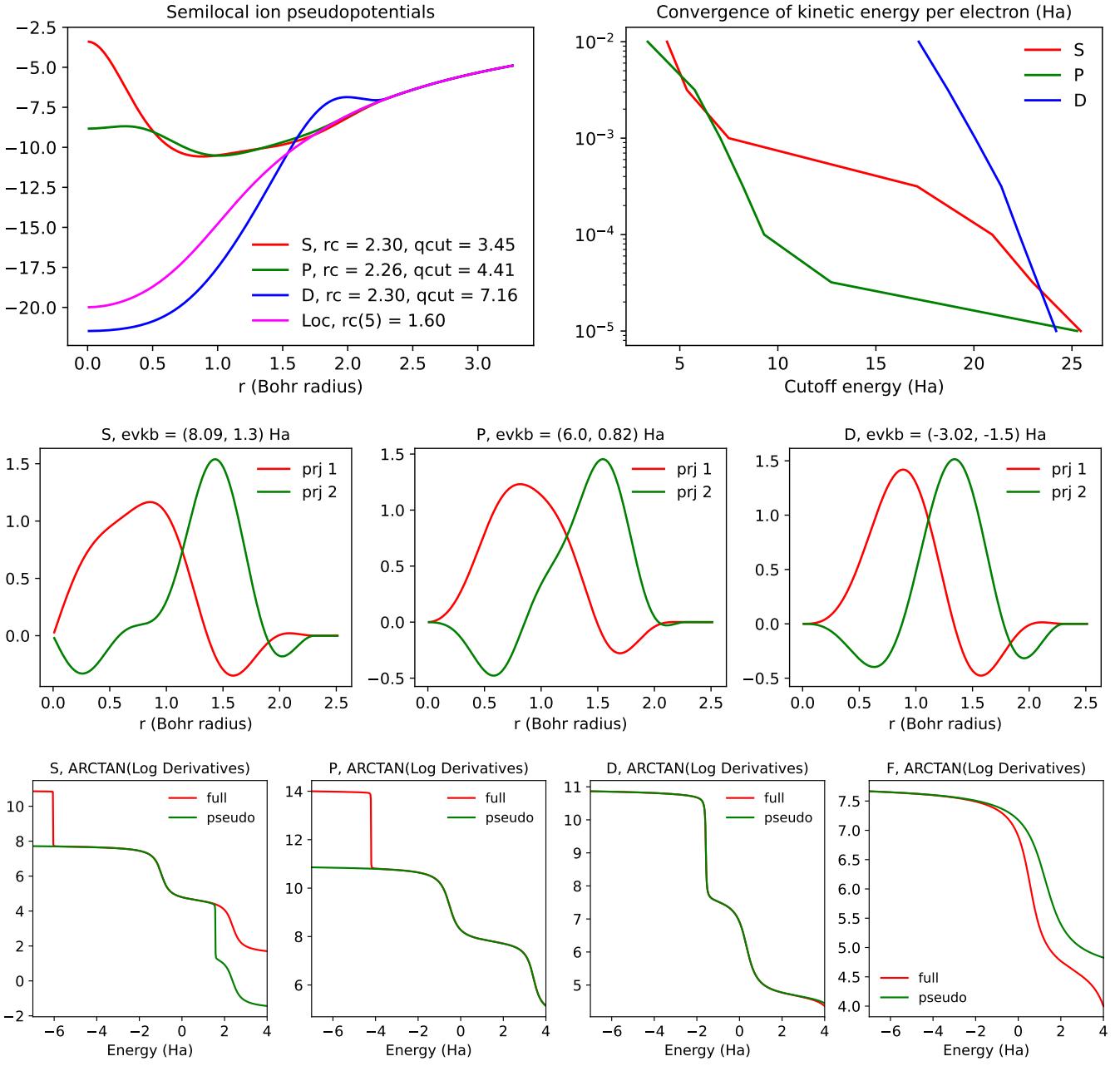
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 16                   | 18                   | 4.16                | 0.89     | 2.05      | 0.06                  | 0.06 | 0.08 | 0.50                  | 0.50 | 0.10              | 0.10 |
| PseudoDojo | 31                   | 34                   | 3.77                | 0.77     | 1.76      | 0.00                  | 0.01 | 0.07 | 0.76                  | 0.76 | 0.03              | 0.03 |
| SG15       | 17                   | 21                   | 3.94                | 0.46     | 1.05      | 0.03                  | 0.04 | 0.07 | 0.97                  | 0.97 | 0.01              | 0.01 |

# Antimony (Sb)



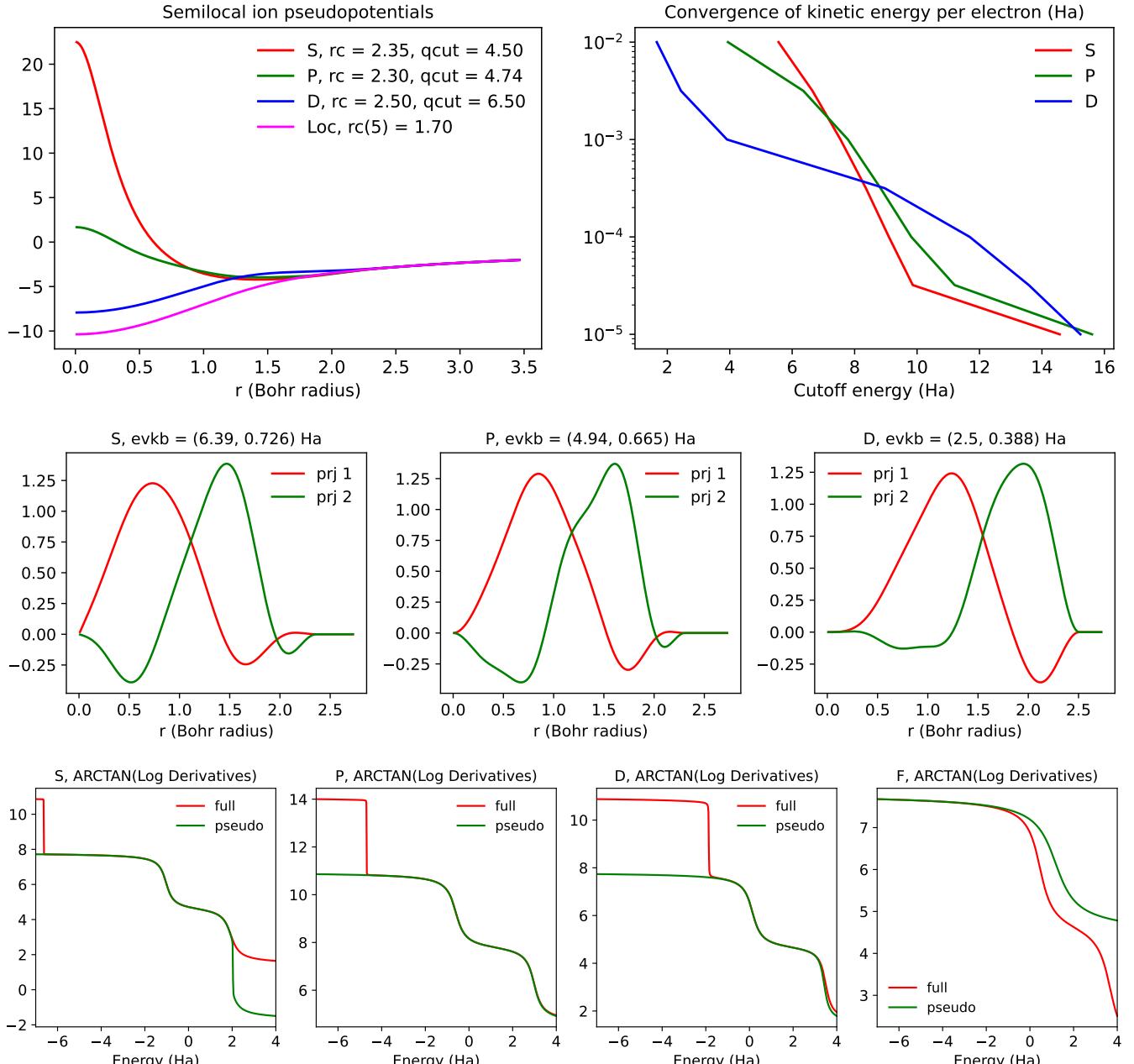
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 22                   | 24                   | 0.69                | 0.42     | 0.78      | 0.01                  | 0.03 | 0.06 | 0.25                  | 0.13 | 0.14              | 0.00 |
| PseudoDojo | 35                   | 38                   | 1.70                | 0.53     | 1.00      | 0.04                  | 0.05 | 0.06 | 0.13                  | 0.05 | 0.01              | 0.07 |
| SG15       | 20                   | 26                   | 2.34                | 0.43     | 0.81      | 0.05                  | 0.07 | 0.05 | 0.28                  | 0.15 | 0.11              | 0.05 |

# Tellurium (Te)



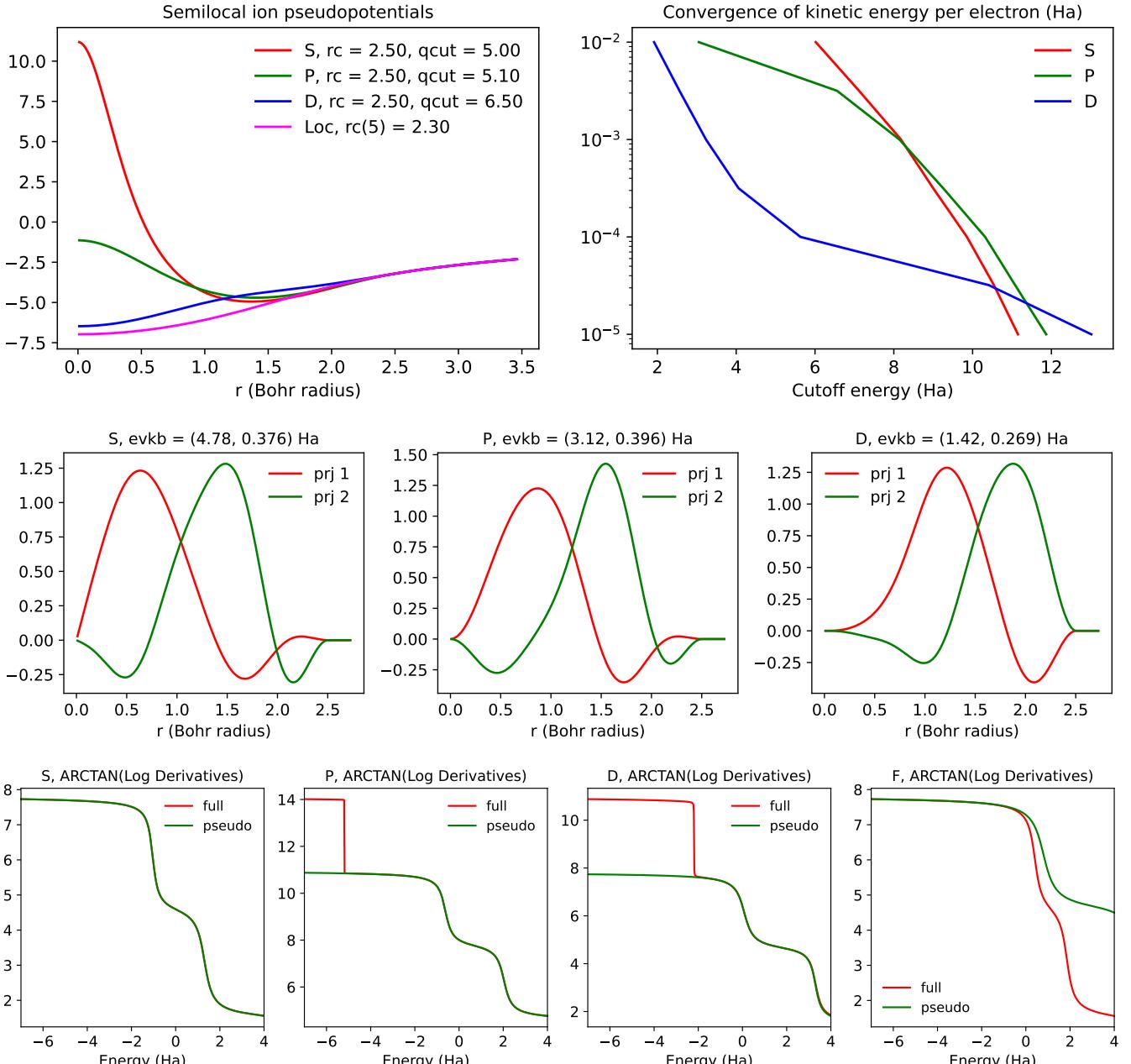
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 22                   | 25                   | 2.23                | 0.43     | 0.82      | 0.07                  | 0.11 | 0.12 | 0.14                  | 0.12 | 0.01              | 0.02 |
| PseudoDojo | 32                   | 42                   | 2.83                | 0.83     | 1.59      | 0.11                  | 0.16 | 0.11 | 0.13                  | 0.13 | 0.01              | 0.02 |
| SG15       | 22                   | 26                   | 2.92                | 0.96     | 1.83      | 0.12                  | 0.17 | 0.15 | 0.87                  | 0.87 | 0.00              | 0.08 |

# Iodine (I)



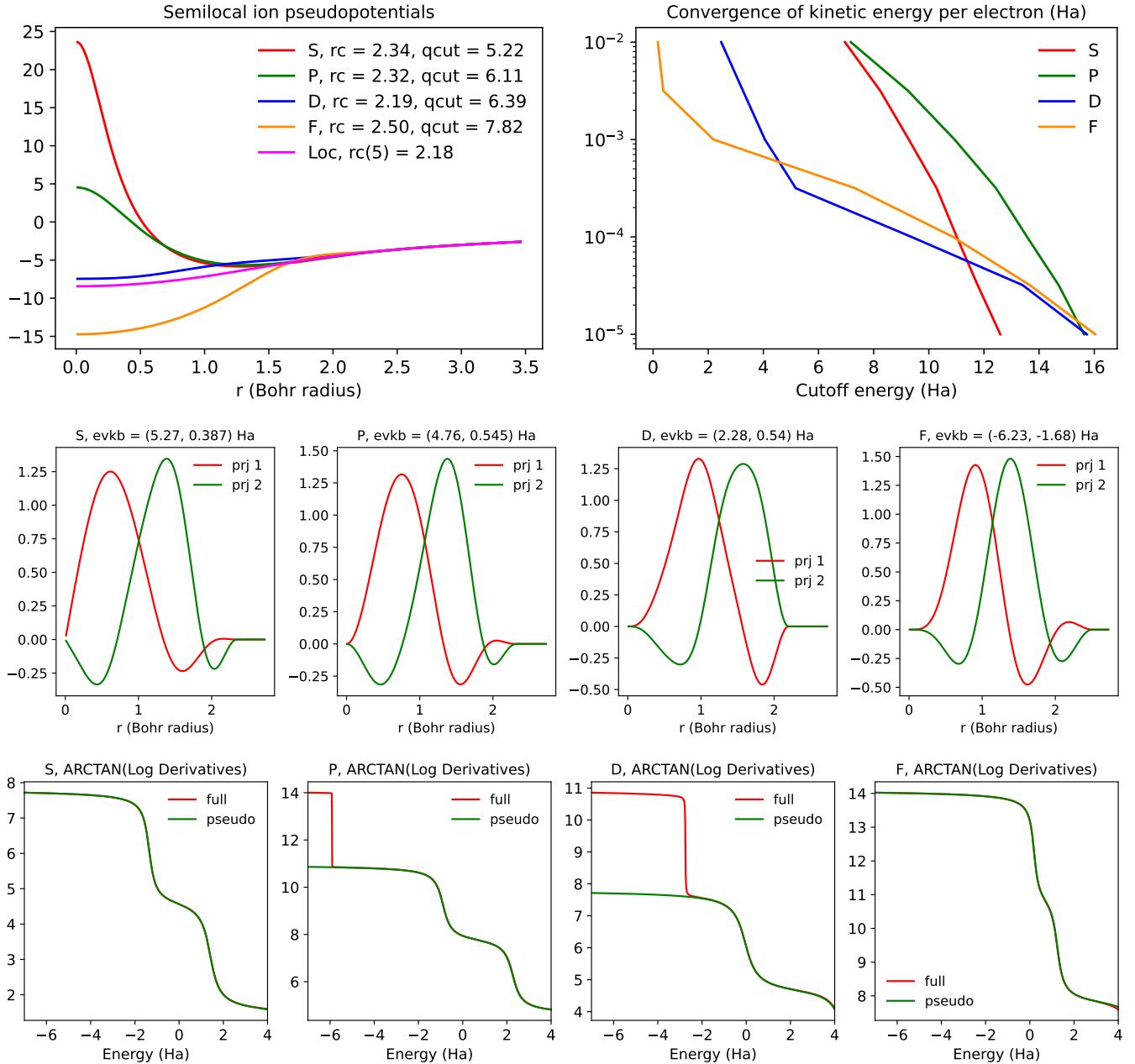
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 9                    | 14                   | 2.09                | 0.02     | 0.08      | 0.08                  | 0.04 | 0.03 | 0.1                   | 0.13 | 1.03              | 0.58 |
| PseudoDojo | 25                   | 31                   | 2.15                | 0.36     | 1.14      | 0.12                  | 0.09 | 0.11 | -                     | -    | -                 | -    |
| SG15       | 24                   | 30                   | 1.54                | 0.73     | 2.33      | 0.15                  | 0.12 | 0.09 | -                     | -    | -                 | -    |

# Xenon (Xe)



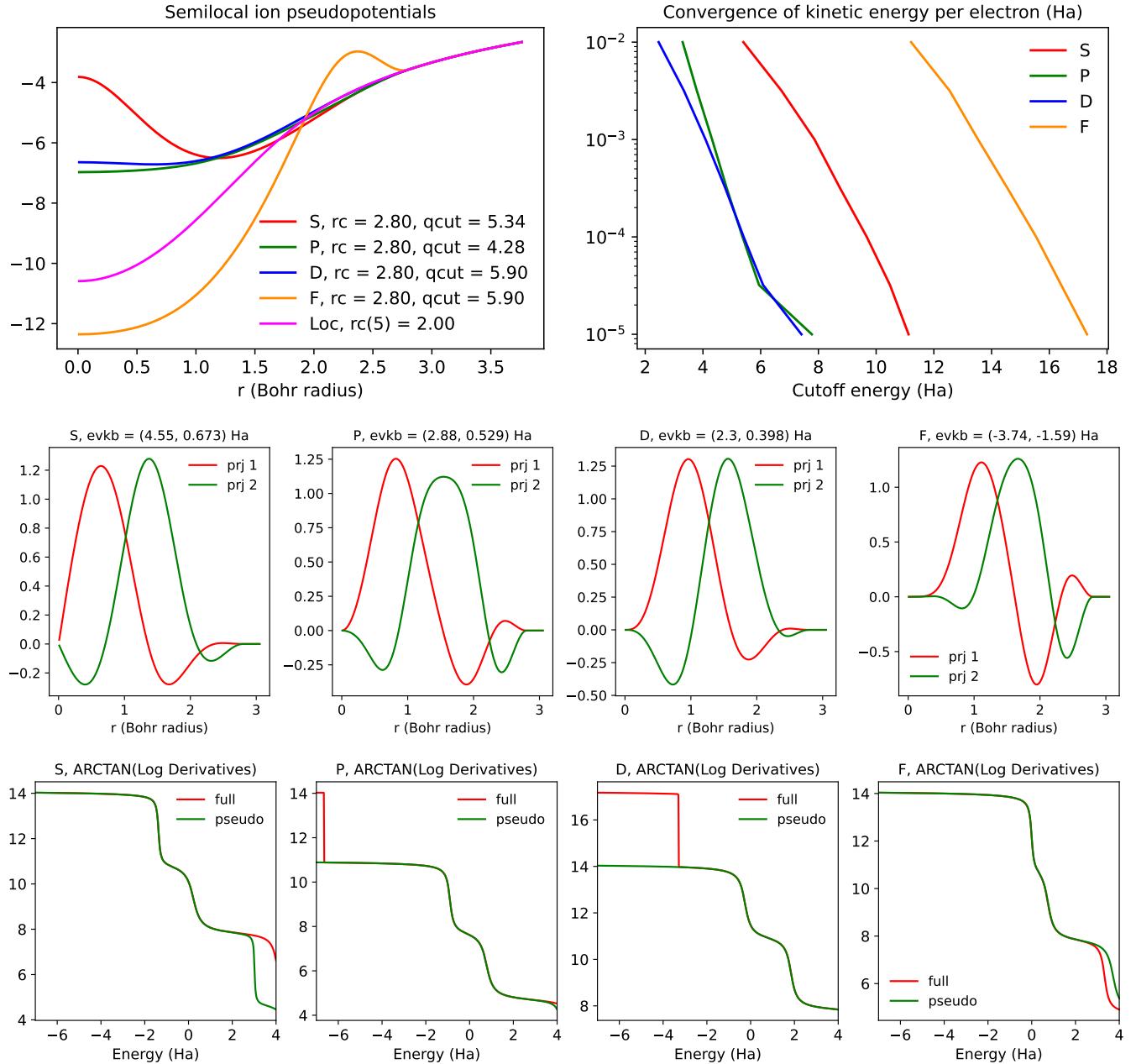
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |     |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|-----|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 10                   | 12                   | 0.84                | 0.05     | 2.90      | -                     | -   | -    | 0.08                  | 0.08 | 4.01              | 4.10 |
| PseudoDojo | 16                   | 31                   | 0.85                | 0.03     | 2.22      | -                     | -   | -    | 0.08                  | 0.08 | 0.87              | 0.75 |
| SG15       | 21                   | 25                   | 0.84                | 0.04     | 2.84      | -                     | -   | -    | -                     | -    | -                 | -    |

# Cesium (Cs)



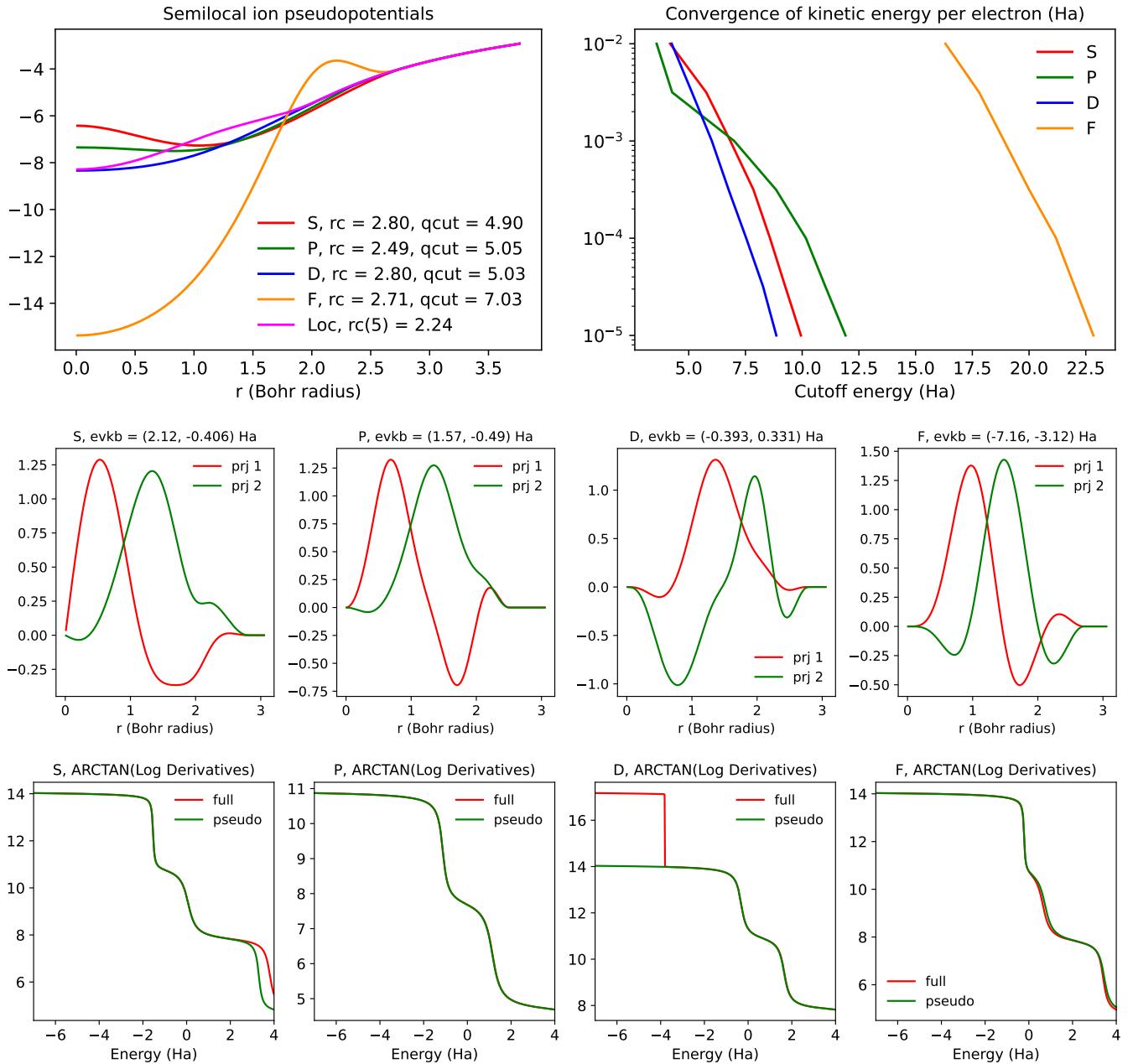
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 13                   | 15                   | 9.33                | 0.12     | 1.56      | 1.34                  | 1.07 | 0.09 | 0.09                  | 0.09 | 0.11              | 0.11 |
| PseudoDojo | 14                   | 18                   | 9.32                | 0.12     | 1.54      | 1.34                  | 1.07 | 0.10 | 0.04                  | 0.04 | 0.03              | 0.03 |
| SG15       | 16                   | 19                   | 9.28                | 0.09     | 1.26      | 1.32                  | 1.06 | 0.10 | 0.35                  | 0.35 | 0.02              | 0.02 |

# Barium (Ba)



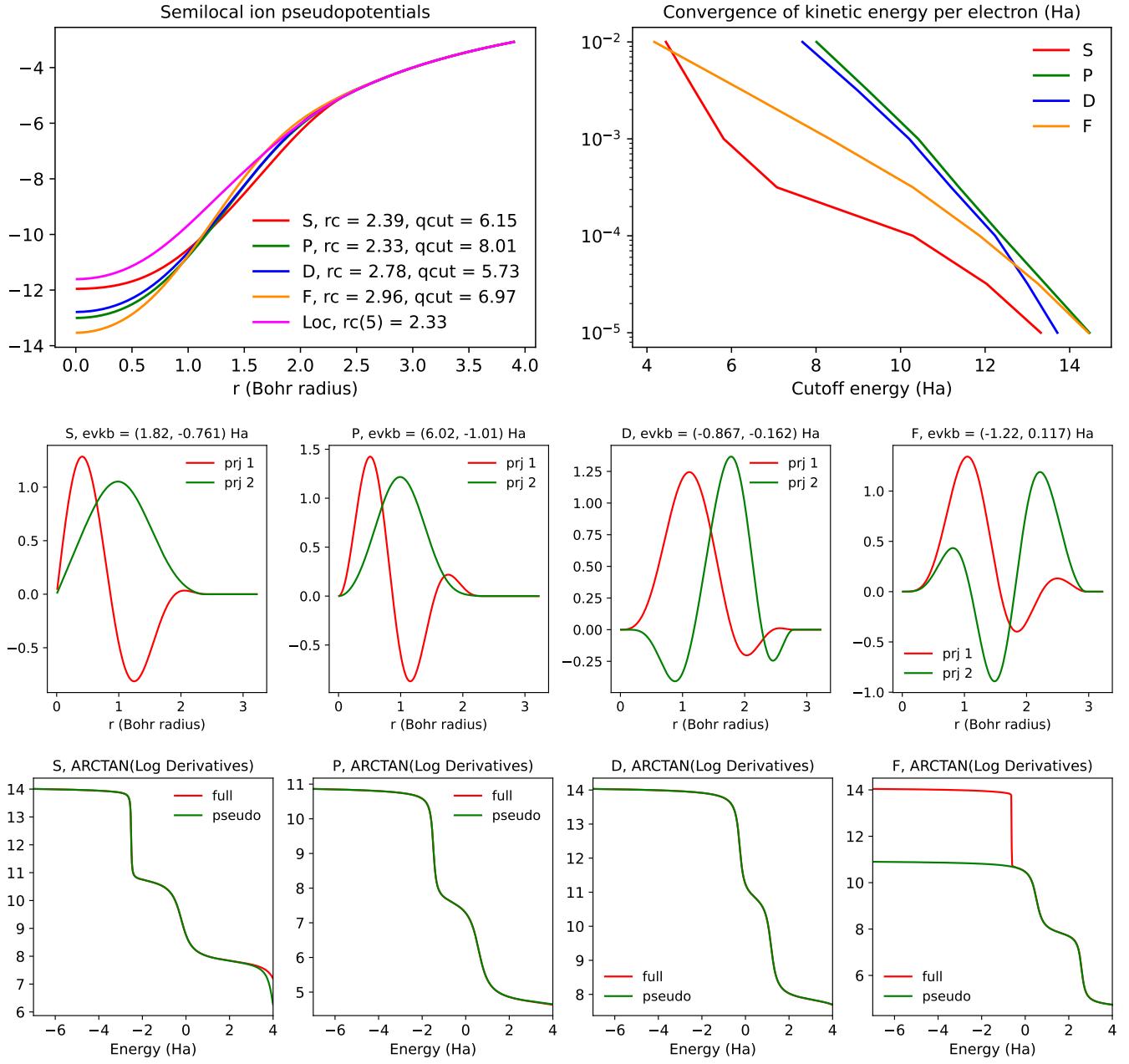
|            | $E_{cut}$            |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{lat}$ |      |      | $\delta_{asr}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|----------------|------|------|----------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC            | FCC  | COMP | LAP            | HAP  | LOP               | HOP  |
| SPMS       | 8                    | 11                   | 0.85                | 0.33     | 1.82      | 0.09           | 0.08 | 0.10 | 0.07           | 0.07 | 0.01              | 0.01 |
| PseudoDojo | 16                   | 19                   | 0.85                | 0.91     | 4.93      | 0.07           | 0.07 | 0.15 | 0.28           | 0.28 | 0.02              | 0.02 |
| SG15       | 9                    | 14                   | 0.74                | 0.40     | 2.20      | 0.07           | 0.08 | 0.08 | 0.14           | 0.14 | 0.17              | 0.17 |

# Lanthanum (La)



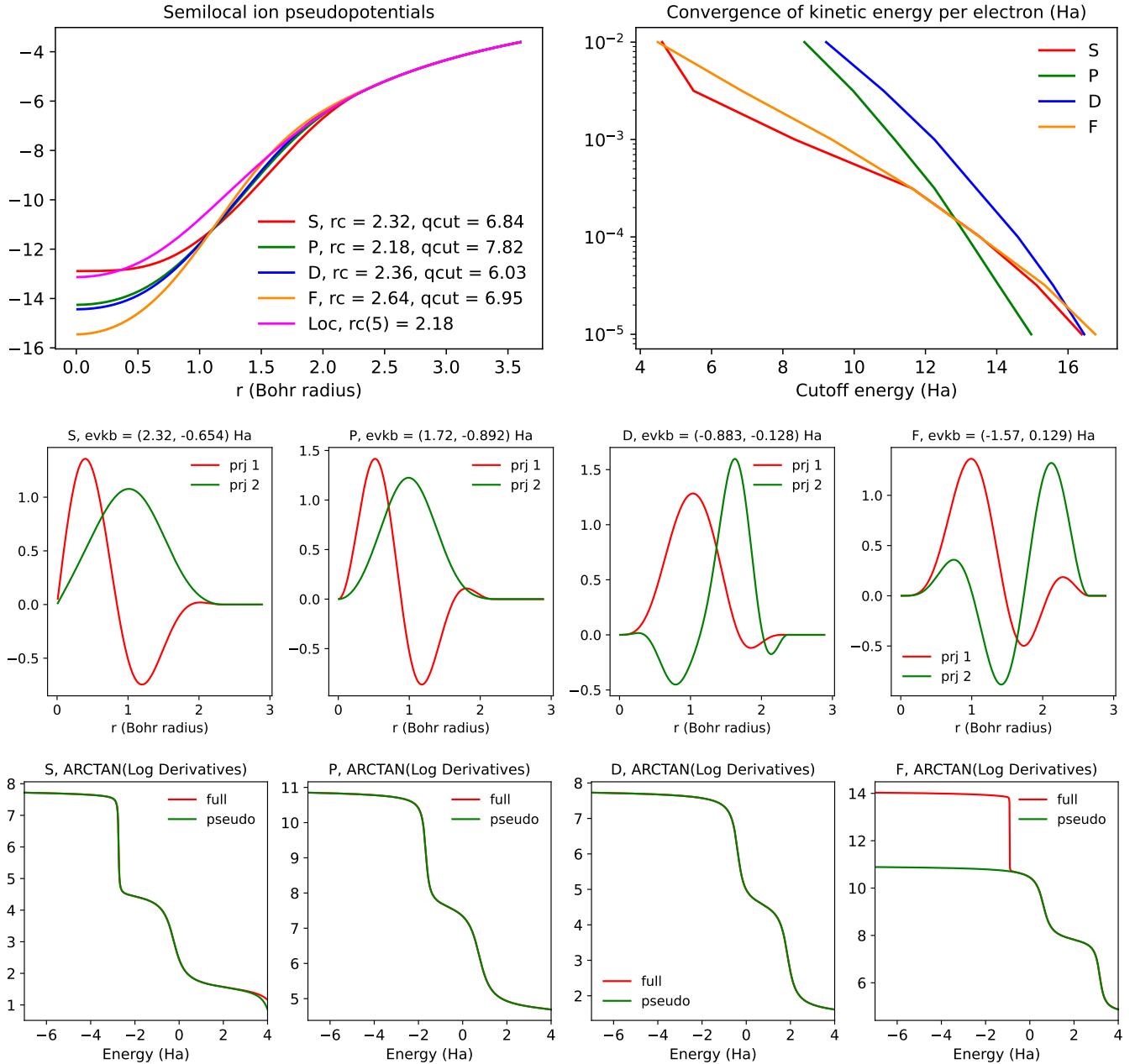
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |     | $\delta_{\omega}$ |     |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|-----|-------------------|-----|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP | LOP               | HOP |
| SPMS       | 15                   | 18                   | 1.73                | -        | -         | 0.04                  | 0.02 | 0.09 | -                     | -   | -                 | -   |
| PseudoDojo | 38                   | 47                   | 2.77                | -        | -         | 0.10                  | 0.12 | 0.09 | -                     | -   | -                 | -   |
| SG15       | 20                   | 23                   | 3.11                | -        | -         | 0.14                  | 0.17 | 0.05 | -                     | -   | -                 | -   |

# Hafnium (Hf)



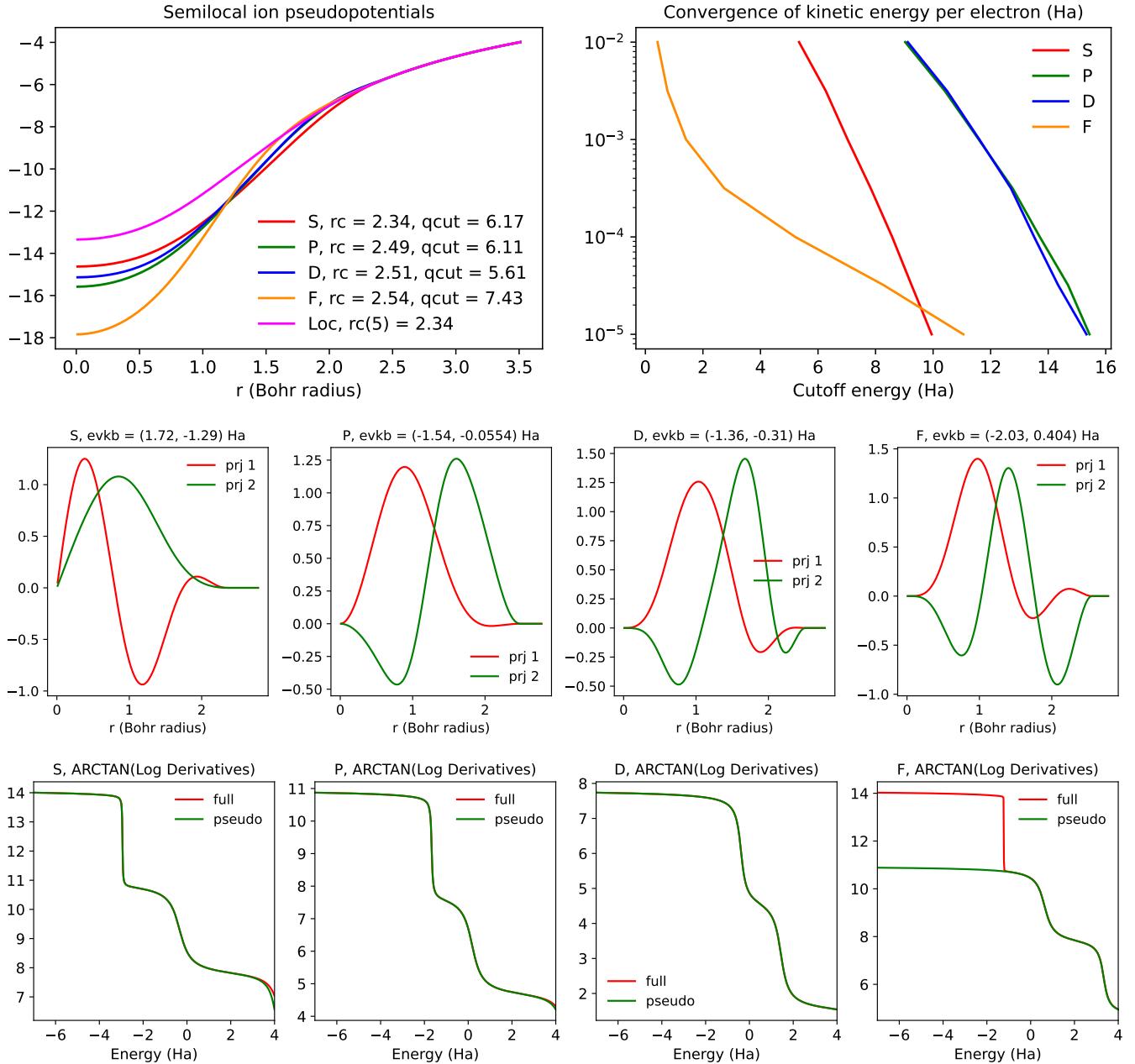
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 12                   | 15                   | 2.82                | 0.40     | 0.50      | 0.03                  | 0.09 | 0.20 | 0.08                  | 0.36 | 0.03              | 0.04 |
| PseudoDojo | 23                   | 28                   | 2.02                | 0.62     | 0.76      | 0.02                  | 0.08 | 0.20 | 0.40                  | 0.25 | 0.03              | 0.04 |
| SG15       | 26                   | 30                   | 7.27                | 1.84     | 2.26      | 0.04                  | 0.01 | 0.11 | -                     | -    | -                 | -    |

# Tantalum (Ta)



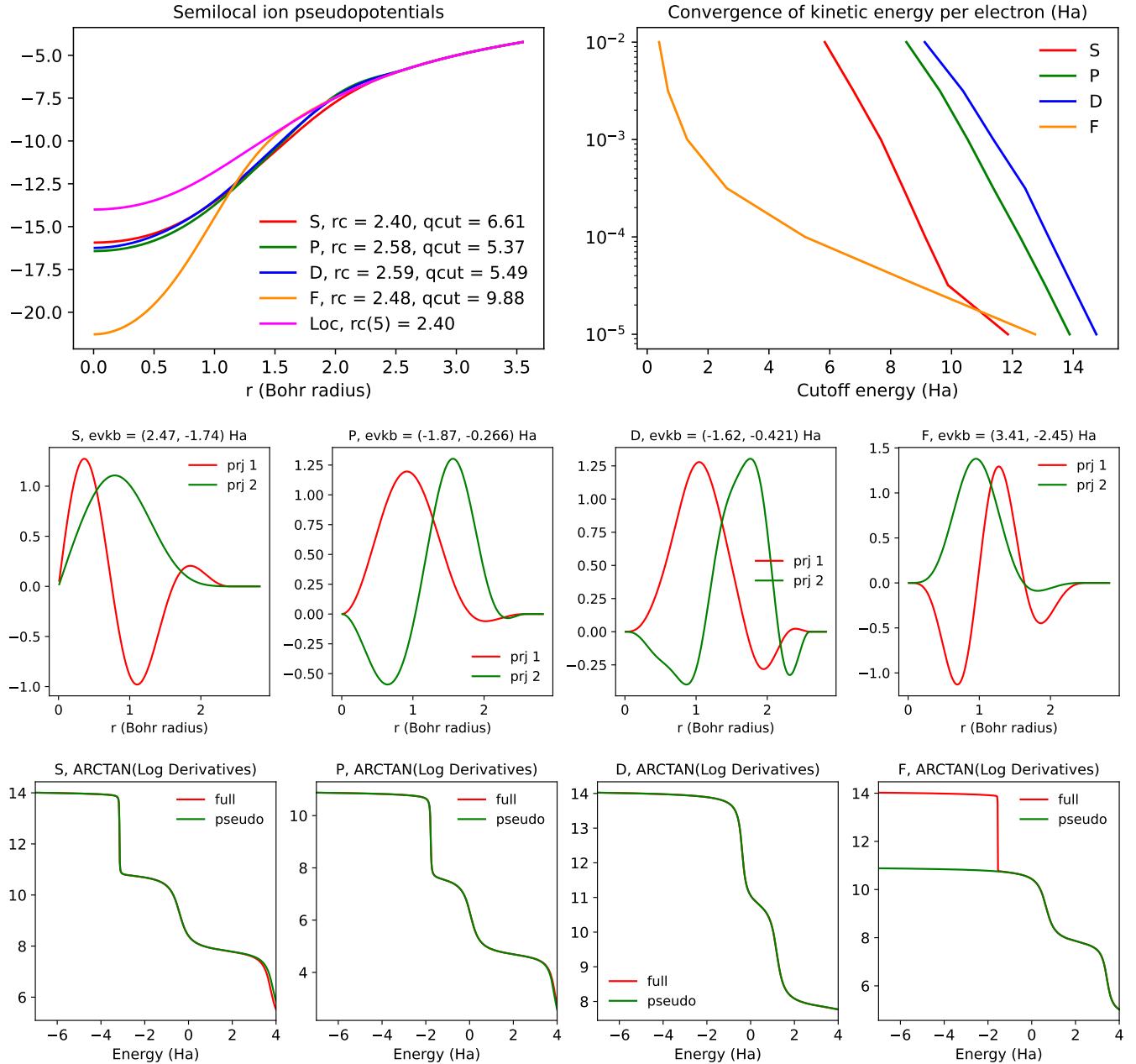
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 14                   | 17                   | 1.52                | 0.67     | 0.57      | 0.22                  | 0.22 | 0.10 | 0.13                  | 0.13 | 0.01              | 0.01 |
| PseudoDojo | 22                   | 28                   | 1.25                | 0.74     | 0.62      | 0.22                  | 0.22 | 0.12 | 0.40                  | 0.40 | 0.01              | 0.01 |
| SG15       | 22                   | 24                   | 5.78                | 2.54     | 2.14      | 0.29                  | 0.30 | 0.10 | -                     | -    | -                 | -    |

# Tungsten (W)



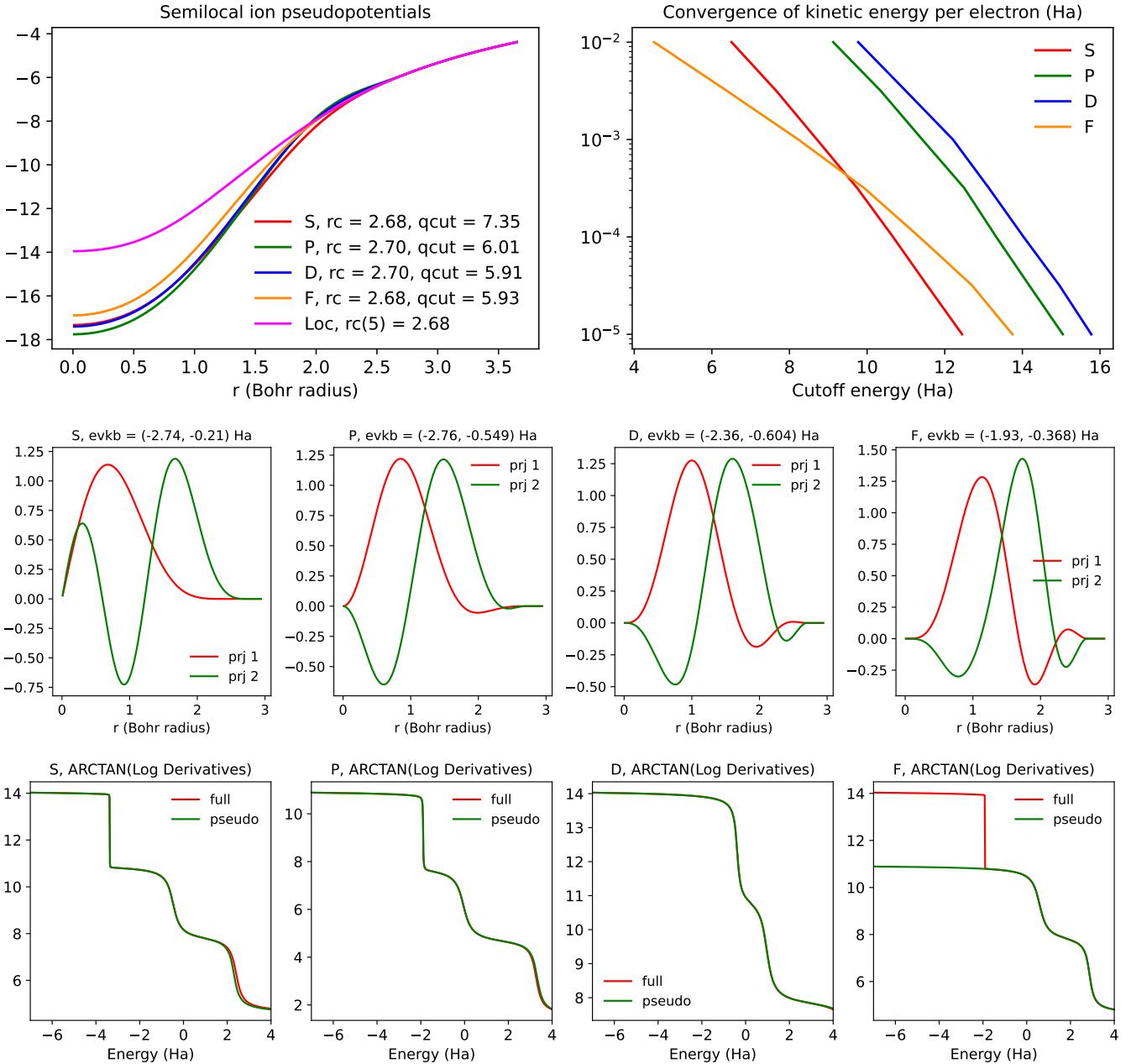
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 13                   | 16                   | 3.68                | 0.14     | 0.08      | 0.31                  | 0.30 | 0.15 | 0.46                  | 0.46 | 0.09              | 0.09 |
| PseudoDojo | 27                   | 42                   | 3.01                | 0.29     | 0.18      | 0.30                  | 0.29 | 0.18 | 0.34                  | 0.34 | 0.09              | 0.09 |
| SG15       | 22                   | 25                   | 2.16                | 0.66     | 0.41      | 0.33                  | 0.35 | 0.21 | -                     | -    | -                 | -    |

# Rhenium (Re)



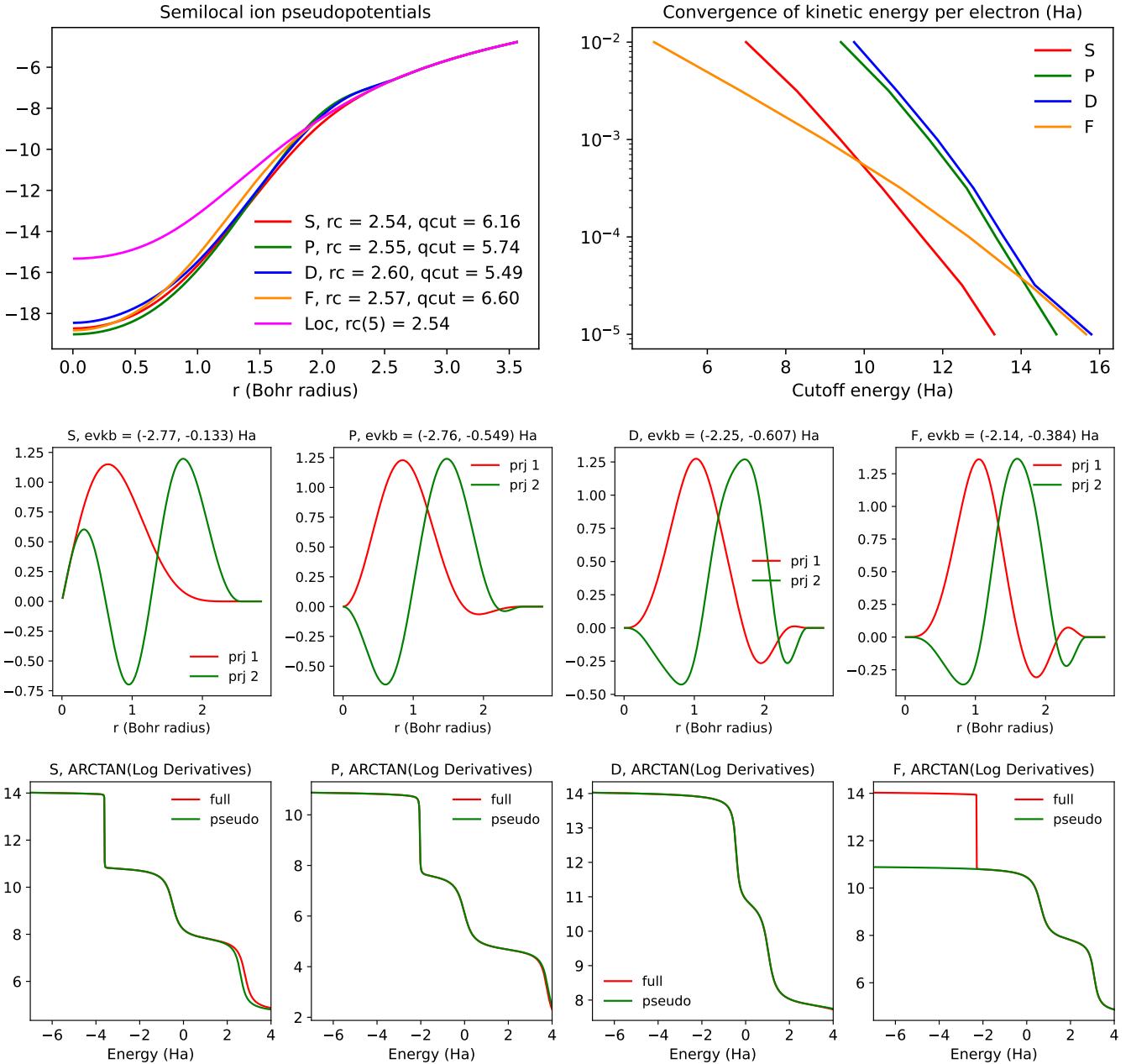
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 13                   | 16                   | 2.89                | 0.34     | 0.19      | 0.22                  | 0.19 | 0.16 | 0.25                  | 0.25 | 0.25              | 0.01 |
| PseudoDojo | 26                   | 37                   | 2.80                | 0.73     | 0.40      | 0.22                  | 0.18 | 0.15 | 0.39                  | 0.23 | 0.01              | 0.02 |
| SG15       | 20                   | 33                   | 3.11                | 0.90     | 0.50      | 0.21                  | 0.18 | 0.14 | 0.58                  | 0.69 | 0.08              | 0.00 |

# Osmium (Os)



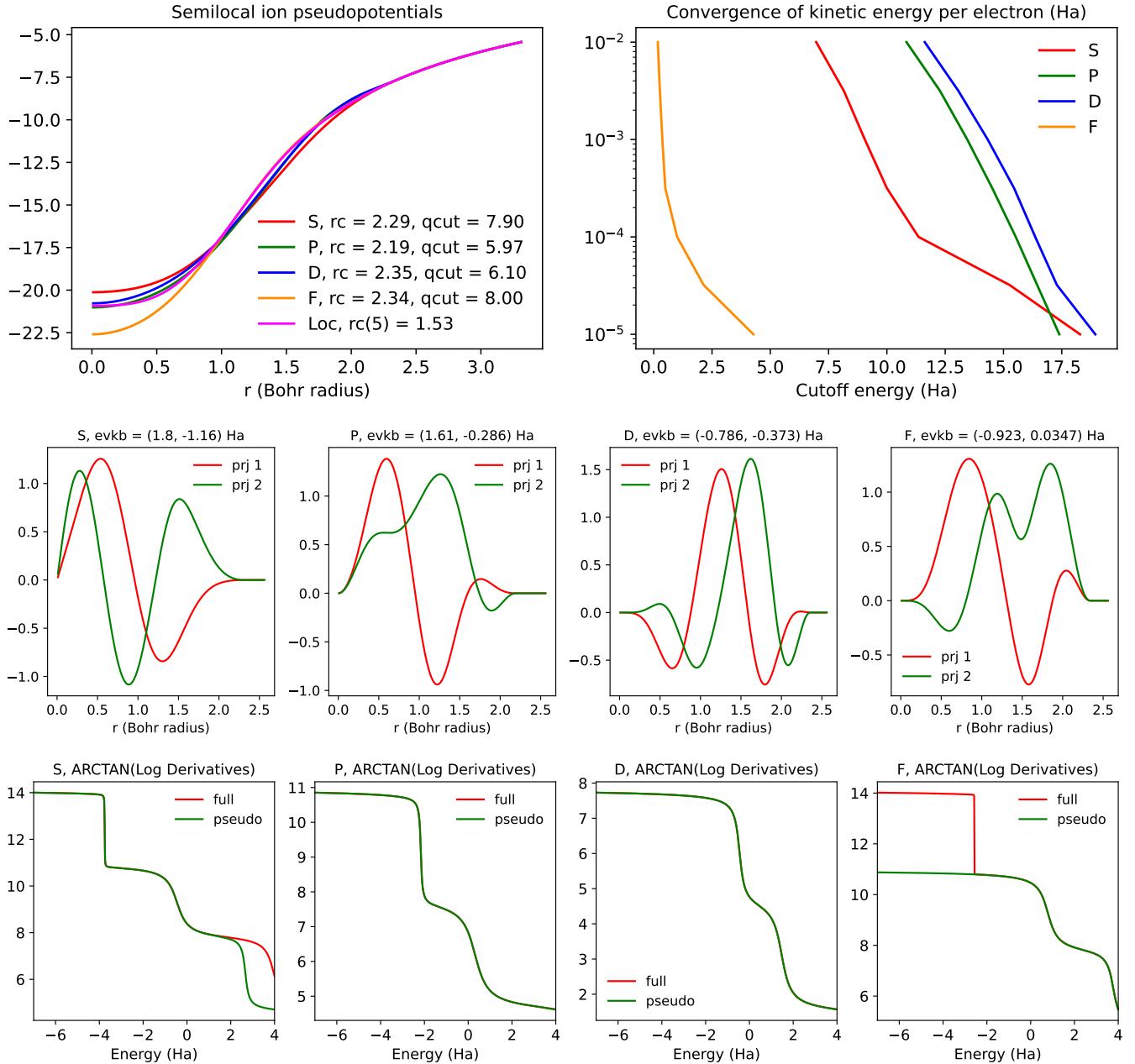
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 14                   | 16                   | 4.26                | 0.33     | 0.18      | 0.21                  | 0.17 | 0.15 | 0.32                  | 0.18 | 0.01              | 0.02 |
| PseudoDojo | 30                   | 34                   | 4.97                | 1.74     | 0.92      | 0.17                  | 0.10 | 0.18 | 0.38                  | 0.22 | 0.00              | 0.00 |
| SG15       | 30                   | 87                   | 4.72                | 1.73     | 0.92      | 0.17                  | 0.10 | 0.16 | 2.49                  | 2.66 | 0.01              | 0.03 |

# Iridium (Ir)



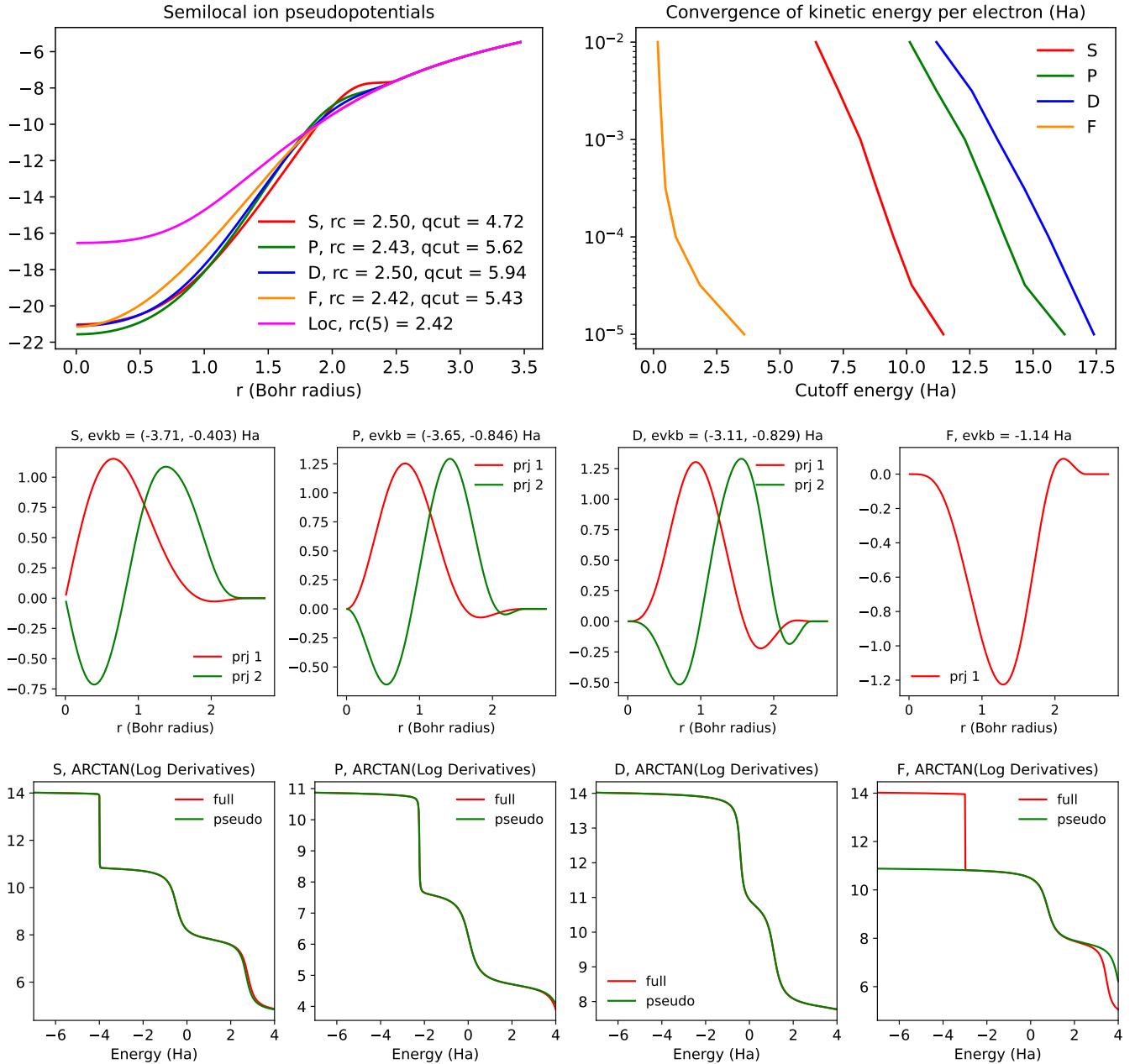
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 13                   | 17                   | 5.15                | 1.00     | 0.60      | 0.07                  | 0.03 | 0.11 | 0.42                  | 0.42 | 0.03              | 0.02 |
| PseudoDojo | 27                   | 33                   | 4.52                | 1.45     | 0.87      | 0.07                  | 0.02 | 0.15 | 0.44                  | 0.44 | 0.01              | 0.00 |
| SG15       | 19                   | 23                   | 4.32                | 1.07     | 0.64      | 0.08                  | 0.03 | 0.12 | 0.06                  | 0.06 | 0.01              | 0.01 |

# Platinum (Pt)



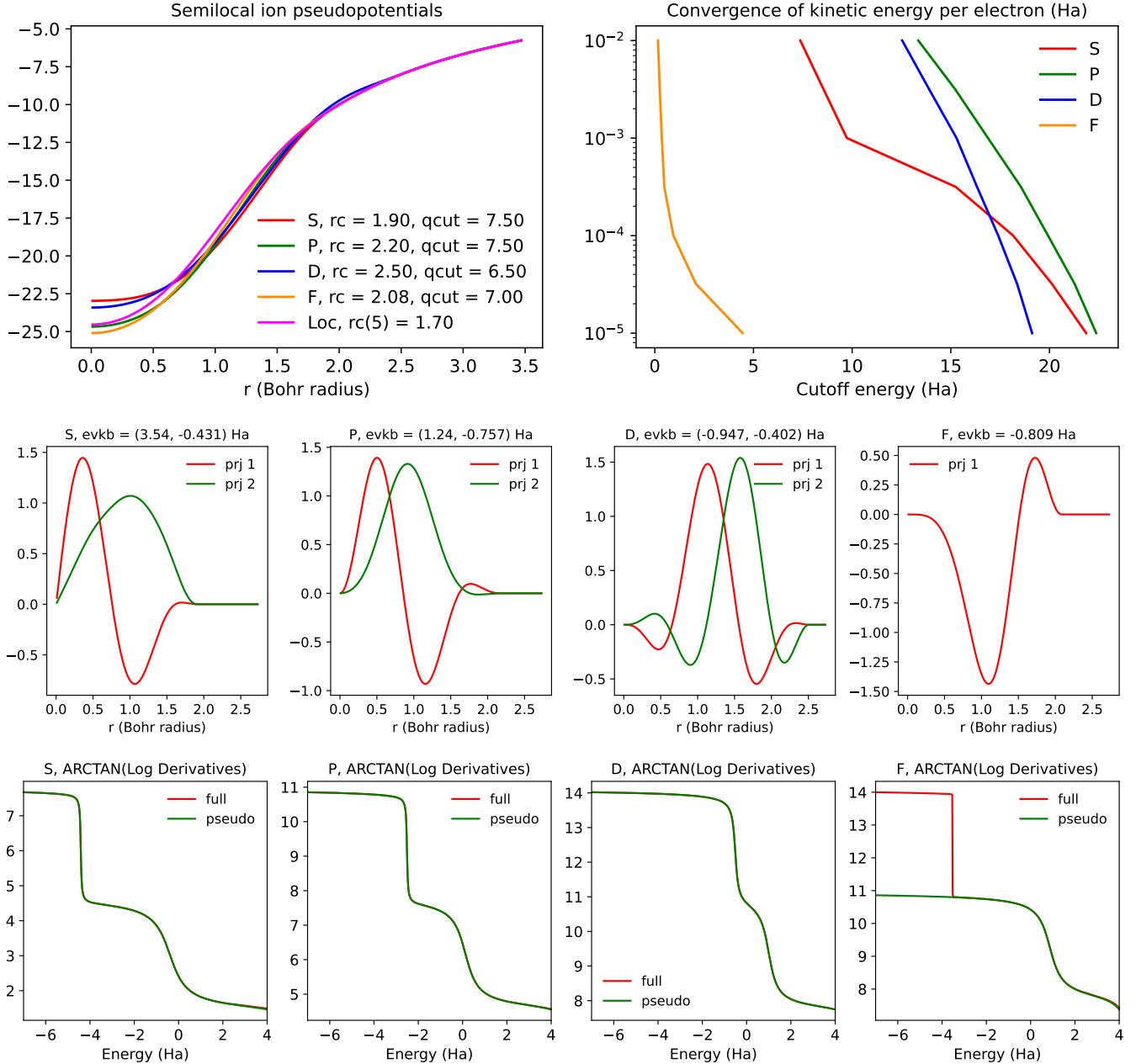
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 17                   | 21                   | 5.19                | 0.16     | 0.12      | 0.03                  | 0.03 | 0.08 | 0.06                  | 0.06 | 0.03              | 0.02 |
| PseudoDojo | 35                   | 40                   | 3.96                | 0.63     | 0.49      | 0.01                  | 0.05 | 0.08 | 0.20                  | 0.20 | 0.03              | 0.02 |
| SG15       | 26                   | 33                   | 6.44                | 3.98     | 3.12      | 0.20                  | 0.13 | 0.07 | 0.11                  | 0.11 | 0.04              | 0.03 |

# Gold (Au)



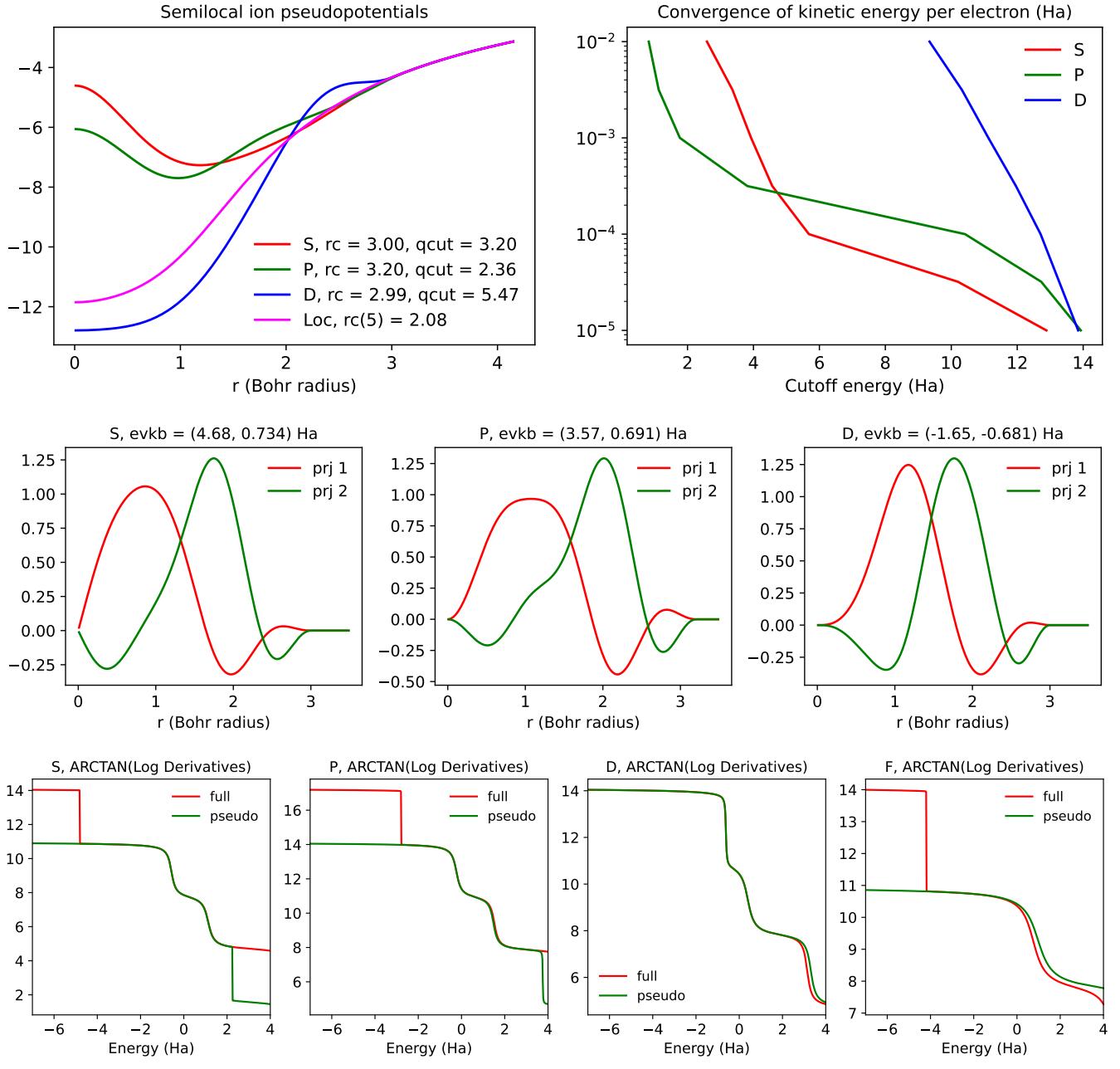
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 16                   | 19                   | 1.48                | 0.21     | 0.24      | 0.05                  | 0.08 | 0.10 | 0.65                  | 0.65 | 0.01              | 0.01 |
| PseudoDojo | 31                   | 35                   | 2.12                | 1.35     | 1.60      | 0.13                  | 0.16 | 0.14 | 0.48                  | 0.48 | 0.04              | 0.02 |
| SG15       | 22                   | 31                   | 2.07                | 0.52     | 0.62      | 0.02                  | 0.05 | 0.12 | 0.49                  | 0.49 | 0.18              | 0.12 |

# Mercury (Hg)



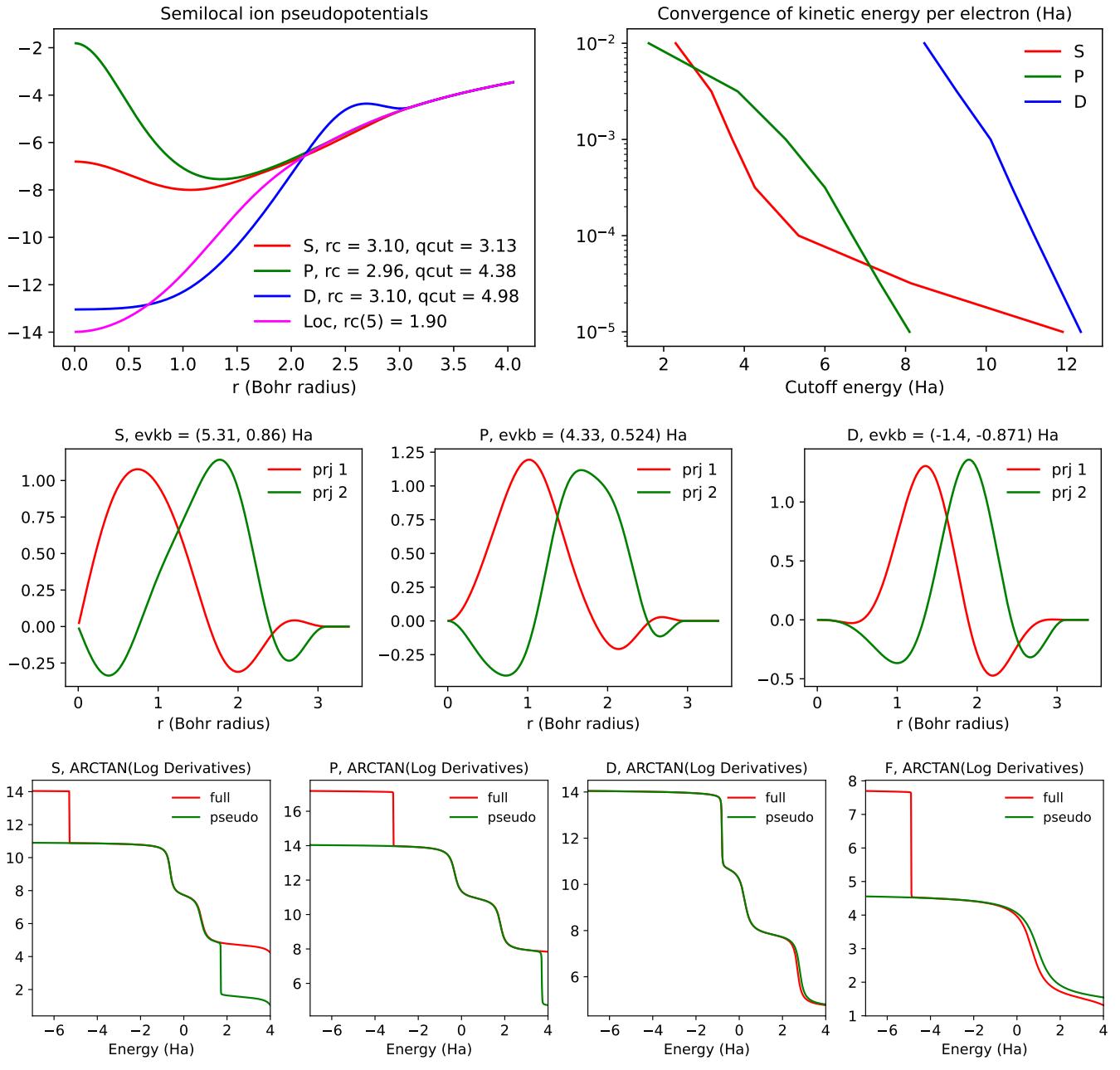
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 20                   | 23                   | 2.35                | 0.77     | 8.24      | 0.08                  | 0.34 | 0.24 | 0.07                  | 0.37 | 0.20              | 0.19 |
| PseudoDojo | 27                   | 32                   | 2.43                | 0.67     | 7.20      | 0.04                  | 0.27 | 0.22 | 0.07                  | 0.15 | 0.21              | 0.06 |
| SG15       | 22                   | 27                   | 2.56                | 0.40     | 4.48      | 0.07                  | 0.13 | 0.19 | 0.23                  | 0.01 | 0.18              | 0.08 |

# Thallium (Tl)



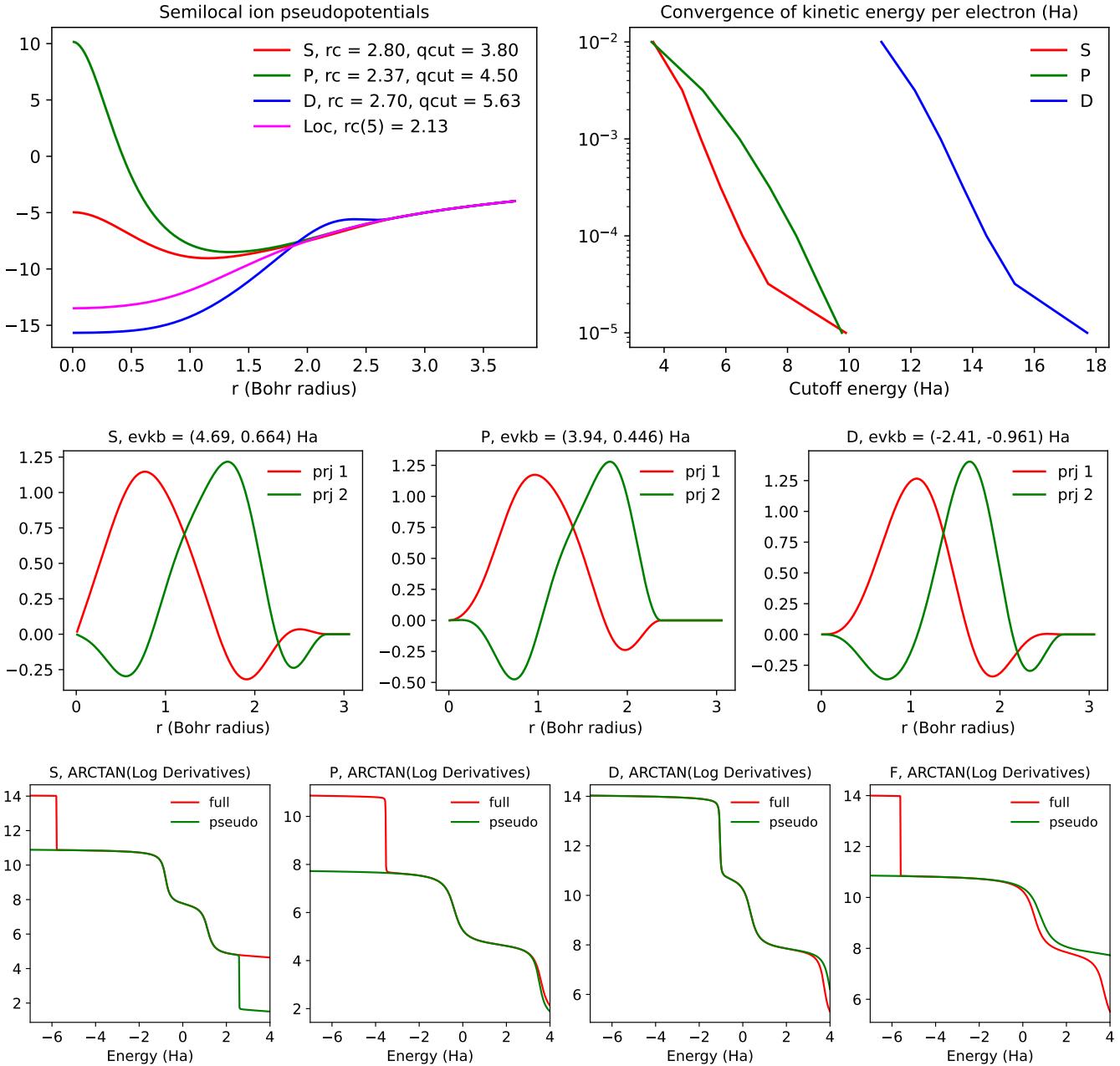
|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 12                   | 14                   | 0.37                | 0.20     | 0.71      | 0.07                  | 0.06 | 0.06 | 0.33                  | 0.34 | 0.50              | 0.39 |
| PseudoDojo | 24                   | 28                   | 0.48                | 0.07     | 0.25      | 0.04                  | 0.02 | 0.05 | 0.45                  | 0.25 | 0.07              | 0.02 |
| SG15       | 15                   | 18                   | 0.36                | 0.17     | 0.60      | 0.06                  | 0.05 | 0.06 | 0.29                  | 0.40 | 0.06              | 0.03 |

# Lead (Pb)



|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 12                   | 14                   | 2.59                | 0.08     | 0.20      | 0.01                  | 0.01 | 0.10 | 0.12                  | 0.12 | 0.05              | 0.07 |
| PseudoDojo | 22                   | 25                   | 2.77                | 0.06     | 0.15      | 0.02                  | 0.01 | 0.15 | 0.07                  | 0.07 | 0.10              | 0.07 |
| SG15       | 14                   | 16                   | 2.88                | 0.07     | 0.17      | 0.02                  | 0.01 | 0.12 | 0.37                  | 0.37 | 0.07              | 0.05 |

Bismuth (Bi)



|            | $E_{\text{cut}}$     |                      | $\delta_{\Delta E}$ | $\Delta$ | $\Delta'$ | $\delta_{\text{lat}}$ |      |      | $\delta_{\text{asr}}$ |      | $\delta_{\omega}$ |      |
|------------|----------------------|----------------------|---------------------|----------|-----------|-----------------------|------|------|-----------------------|------|-------------------|------|
|            | $\delta_E = 10^{-3}$ | $\delta_E = 10^{-4}$ |                     |          |           | BCC                   | FCC  | COMP | LAP                   | HAP  | LOP               | HOP  |
| SPMS       | 14                   | 19                   | 2.79                | 0.42     | 0.79      | 0.00                  | 0.01 | 0.07 | 0.04                  | 0.07 | 0.07              | 0.06 |
| PseudoDojo | 28                   | 31                   | 2.38                | 0.21     | 0.40      | 0.02                  | 0.01 | 0.08 | 0.15                  | 0.14 | 0.01              | 0.03 |
| SG15       | 16                   | 19                   | 1.27                | 0.20     | 0.37      | 0.07                  | 0.06 | 0.07 | 0.20                  | 1.06 | 0.68              | 0.59 |