**Table 4.** The IDs, chemical formulas, PBE band gaps, and HSE06 band gaps for the 75 candidate materials. The predicted HSE06 band gaps of these materials are in the visible wavelength range of 0.9–1.6 eV, which indicates that they may be potential carrier transport layer materials in PSCs.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| ID | Chemical formula | PBE *E*g (eV) | HSE06 *E*g (eV) | ID | Chemical formula | PBE *E*g (eV) | HSE06 *E*g (eV) |
| N-243 | Cu3N | 0.19 | 1.36 | O-658 | FeO2 | 0.87 | 1.02 |
| N-442 | AgN3 | 1.67 | 1.43 | O-660 | Fe2O3 | 1.42 | 1.11 |
| N-488 | HfN2 | 1.39 | 1.07 | O-662 | Fe2O3 | 1.00 | 0.96 |
| N-529 | WN2 | 0.57 | 1.04 | O-665 | Fe2O3 | 0.26 | 1.13 |
| N-534 | WN2 | 0.15 | 0.93 | O-672 | FeO | 0.45 | 1.35 |
| N-546 | WN2 | 0.17 | 1.05 | O-680 | Fe2O3 | 1.08 | 1.29 |
| N-57 | Ti19N25 | 0.01 | 1.30 | O-696 | Fe2O3 | 1.39 | 0.98 |
| N-68 | TiN | 0.01 | 1.13 | O-701 | Fe2O3 | 1.12 | 1.11 |
| N-70 | Ti3N4 | 0.10 | 1.17 | O-704 | FeO2 | 0.95 | 1.10 |
| O-1336 | W3O8 | 1.70 | 1.58 | O-707 | Fe7O9 | 1.14 | 1.17 |
| O-1339 | WO2 | 1.25 | 1.10 | O-716 | Fe2O3 | 0.18 | 1.04 |
| O-1373 | W3O8 | 0.73 | 1.53 | O-718 | Fe2O3 | 0.27 | 1.26 |
| O-1381 | W2O3 | 0.02 | 1.25 | O-733 | Fe43O64 | 0.77 | 0.95 |
| O-1383 | WO2 | 1.73 | 1.54 | O-739 | Fe2O3 | 0.12 | 1.23 |
| O-1396 | WO2 | 2.23 | 1.41 | O-743 | Fe2O3 | 1.41 | 1.18 |
| O-1397 | WO2 | 1.40 | 1.22 | O-744 | Fe2O3 | 2.02 | 0.95 |
| O-1408 | WO2 | 1.40 | 1.41 | O-758 | Fe2O3 | 1.49 | 0.93 |
| O-1409 | WO2 | 1.61 | 1.56 | O-772 | CoO | 0.22 | 1.52 |
| O-1412 | WO2 | 2.47 | 1.46 | O-776 | CoO | 0.35 | 1.57 |
| O-1416 | W3O8 | 1.82 | 1.55 | O-784 | Co29O40 | 0.26 | 1.40 |
| O-1464 | HgO | 1.19 | 1.34 | O-786 | Co23O32 | 0.30 | 1.59 |
| O-1468 | HgO | 1.20 | 1.31 | O-796 | CoO | 0.27 | 1.47 |
| O-1469 | HgO | 1.30 | 1.35 | O-808 | CoO | 0.26 | 1.41 |
| O-1470 | HgO | 1.24 | 1.29 | O-816 | Co2O3 | 0.15 | 0.98 |
| O-407 | VO | 0.81 | 1.45 | O-861 | CuO | 0.15 | 1.39 |
| O-531 | Cr3O4 | 0.97 | 1.20 | O-882 | CuO | 0.01 | 1.39 |
| O-539 | Cr2O3 | 2.43 | 1.52 | O-939 | Rb2O2 | 0.01 | 1.41 |
| O-543 | CrO | 0.17 | 1.45 | S-158 | Fe7S12 | 0.17 | 1.59 |
| O-545 | Cr2O3 | 2.13 | 1.51 | S-168 | FeS2 | 0.46 | 1.58 |
| O-552 | Cr2O3 | 1.77 | 1.57 | S-172 | Fe3S4 | 0.00 | 1.53 |
| O-561 | CrO | 0.50 | 1.22 | S-182 | Fe7S8 | 0.02 | 1.11 |
| O-567 | CrO | 0.34 | 1.09 | S-225 | Cu2S | 0.12 | 1.11 |
| O-570 | CrO2 | 0.34 | 1.60 | S-505 | RuS2 | 0.67 | 1.53 |
| O-584 | Cr9O13 | 0.61 | 1.17 | S-507 | Rh2S3 | 0.42 | 1.03 |
| O-585 | Cr5O7 | 0.78 | 1.17 | S-508 | Rh2S3 | 0.19 | 1.17 |
| O-590 | Cr2O3 | 0.59 | 1.19 | S-635 | HgS | 1.70 | 1.37 |
| O-652 | Fe2O3 | 1.54 | 0.99 | S-639 | HgS | 1.68 | 1.37 |
| O-657 | Fe2O3 | 0.14 | 1.40 |  |  |  |  |