First-principles calculations of opto-electronic and thermoelectric properties double perovskite semiconductors $M_2ScInCl_6$ (M = Rb, Cs)

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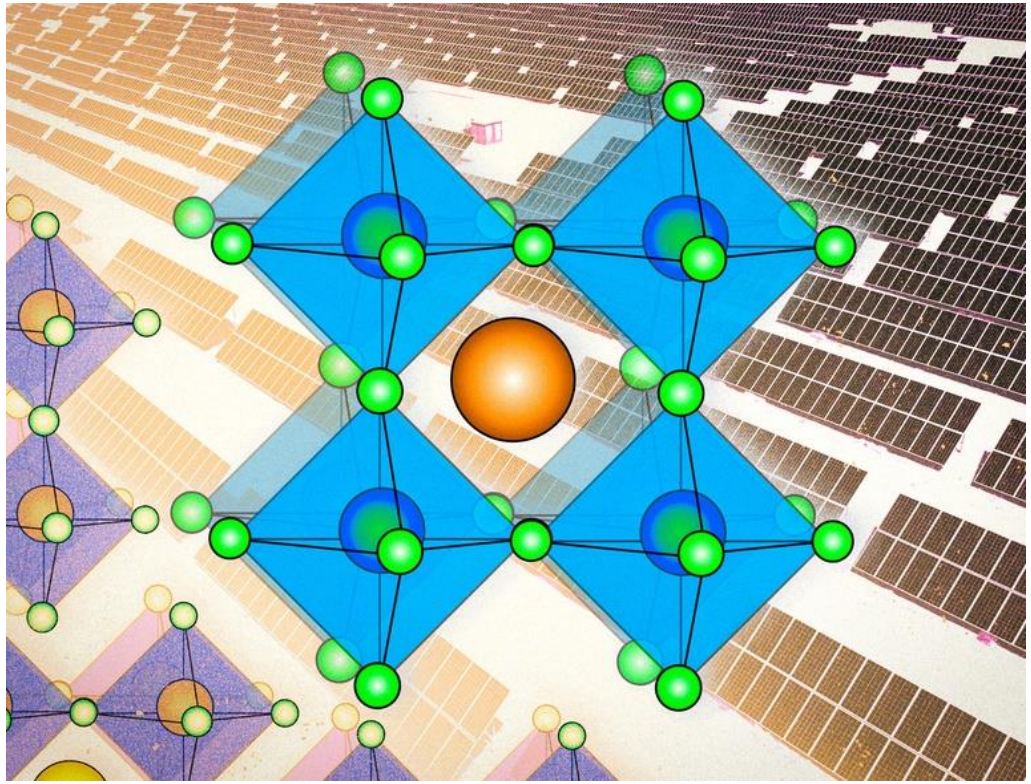
Outline

- Lead-free double perovskite
- Our systems of study: $Rb_2ScInCl_6$ and $Cs_2ScInCl_6$
- Computational details
- Opto-electronic properties
- Thermoelectric properties
- Conclusions

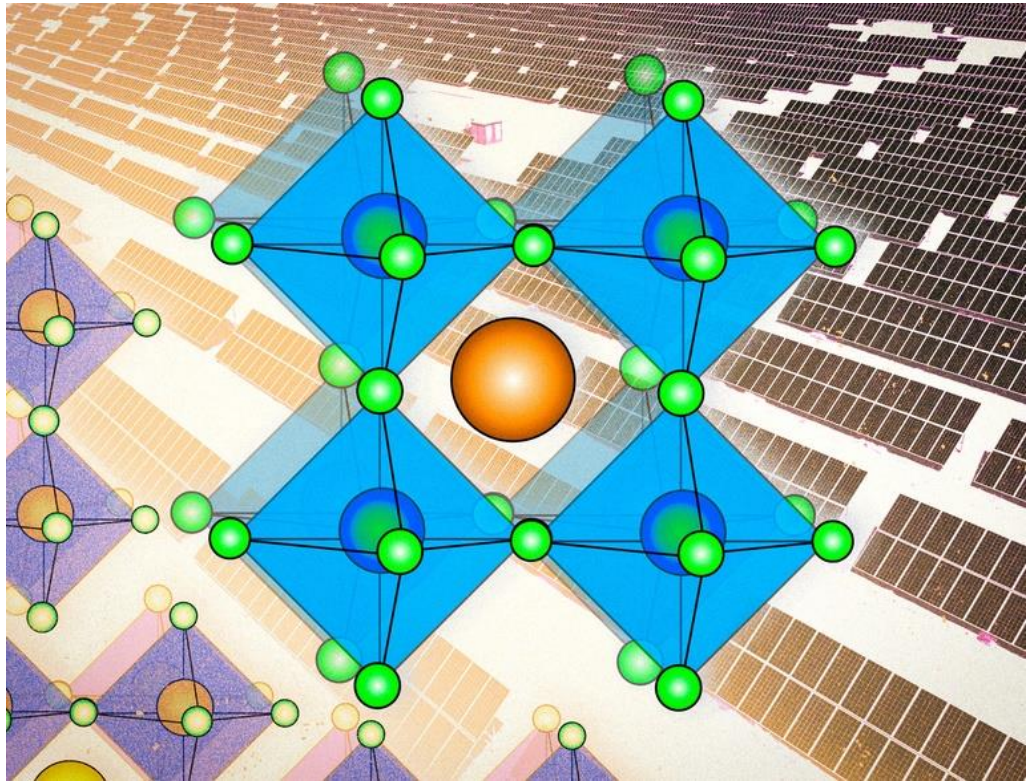
Perovskite solar cells



https://news.mit.edu/2022/perovskites-solar-cells-explained-0715

Perovskite solar cells

- High power conversion efficiency (about 25%)
- Easier manufacturing process
- Lower cost and greater flexibility



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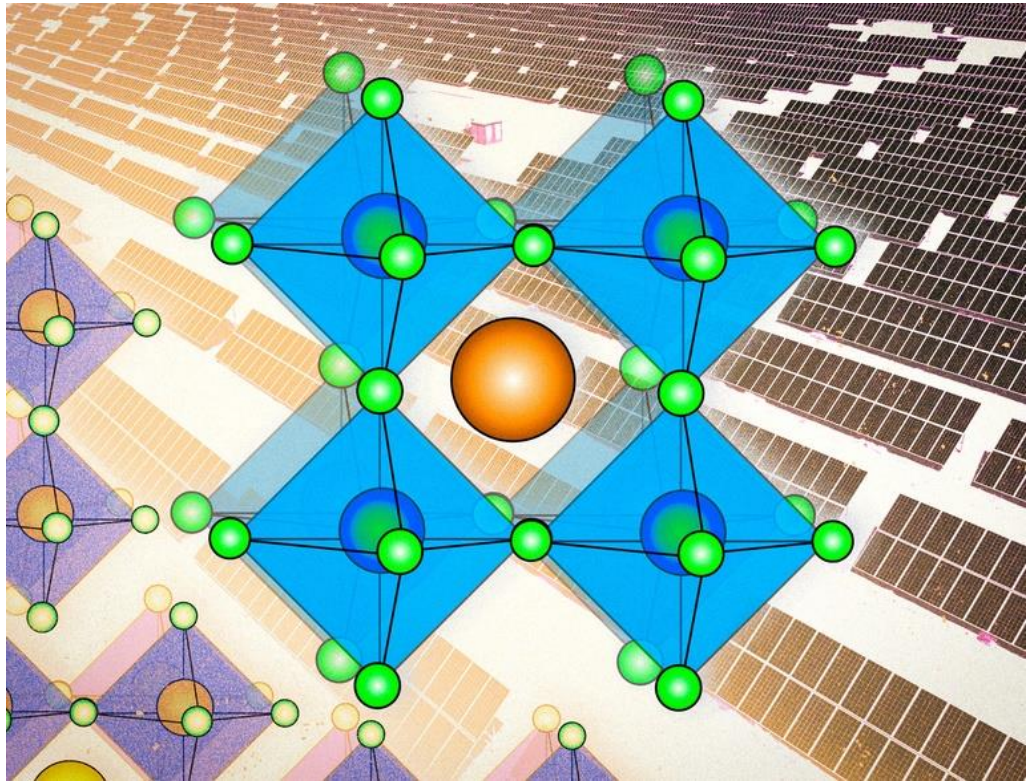
Perovskite solar cells

- High power conversion efficiency (about 25%)
- Easier manufacturing process
- Lower cost and greater flexibility
- Perovskites degrade much faster
- Pb-based perovskites show better potential but they are toxic



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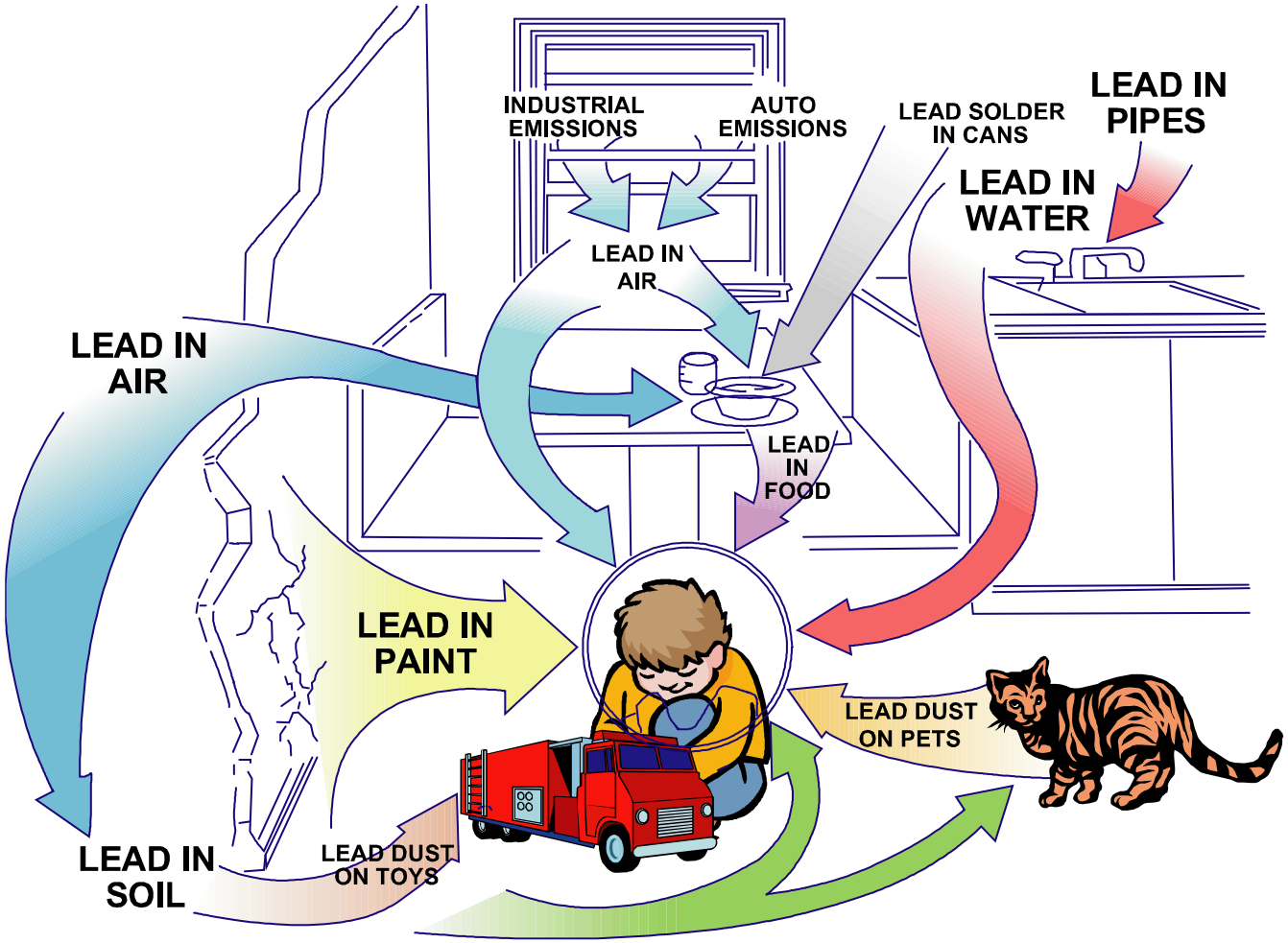
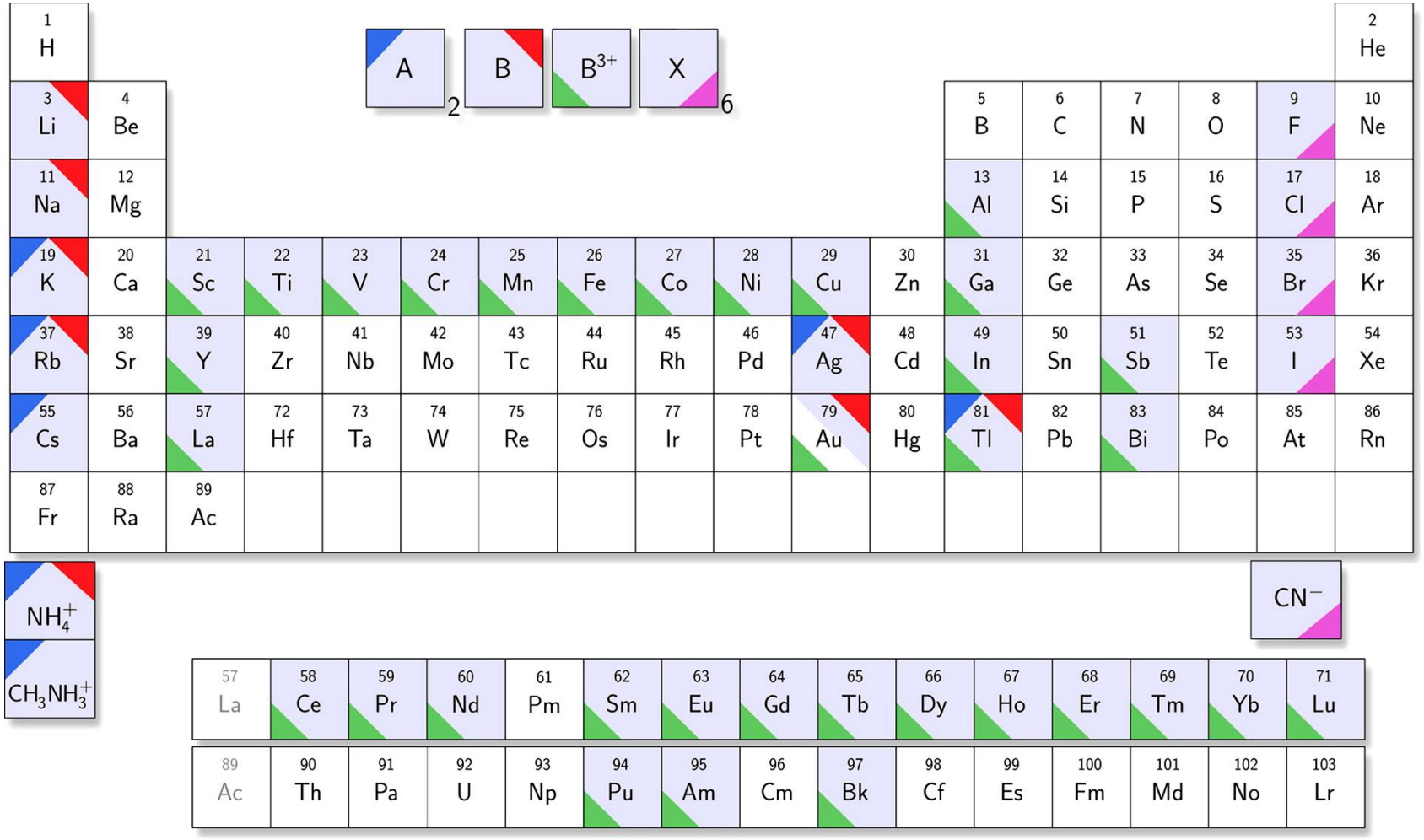
Environmental sources of lead exposure



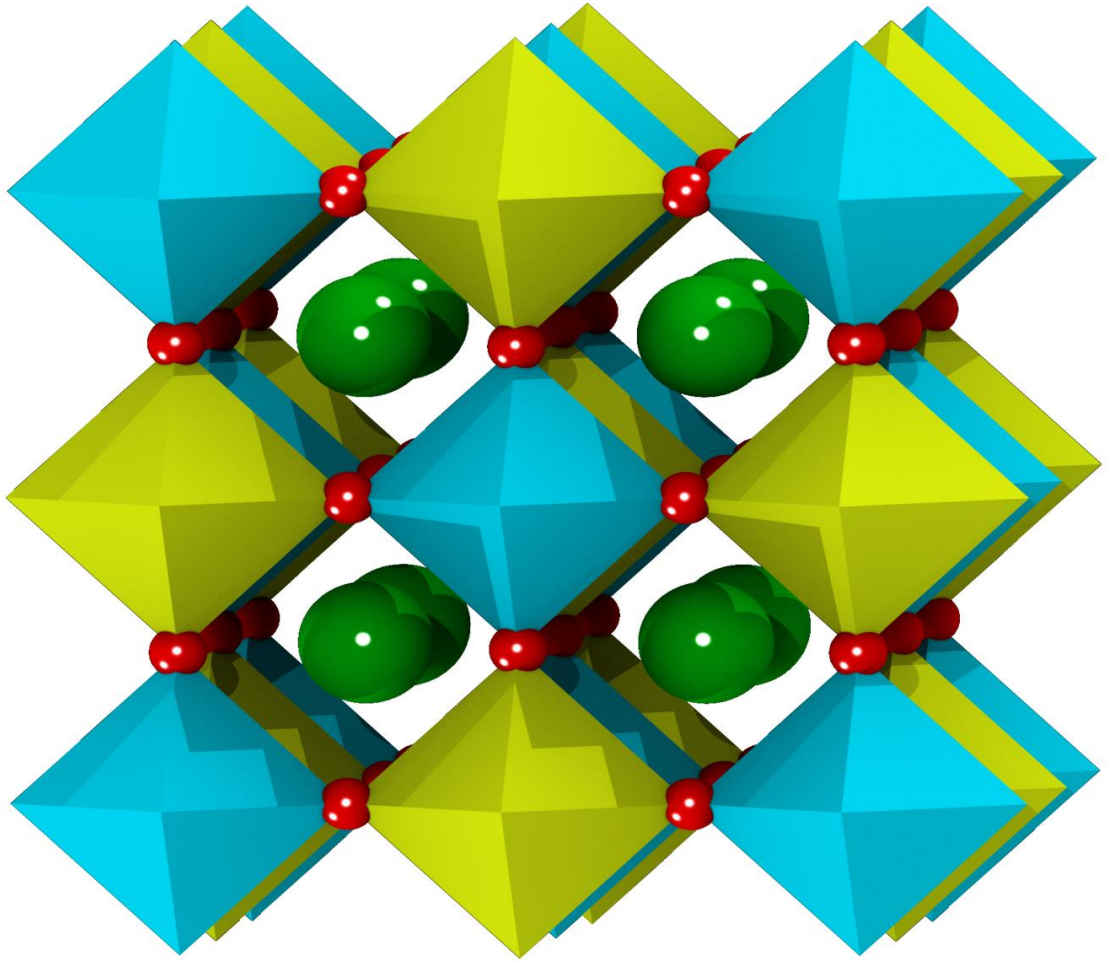
https://www.cdc.gov/nceh/lead/publications/refugeetoolkit/powerpoint_files/medicalservice.ppt

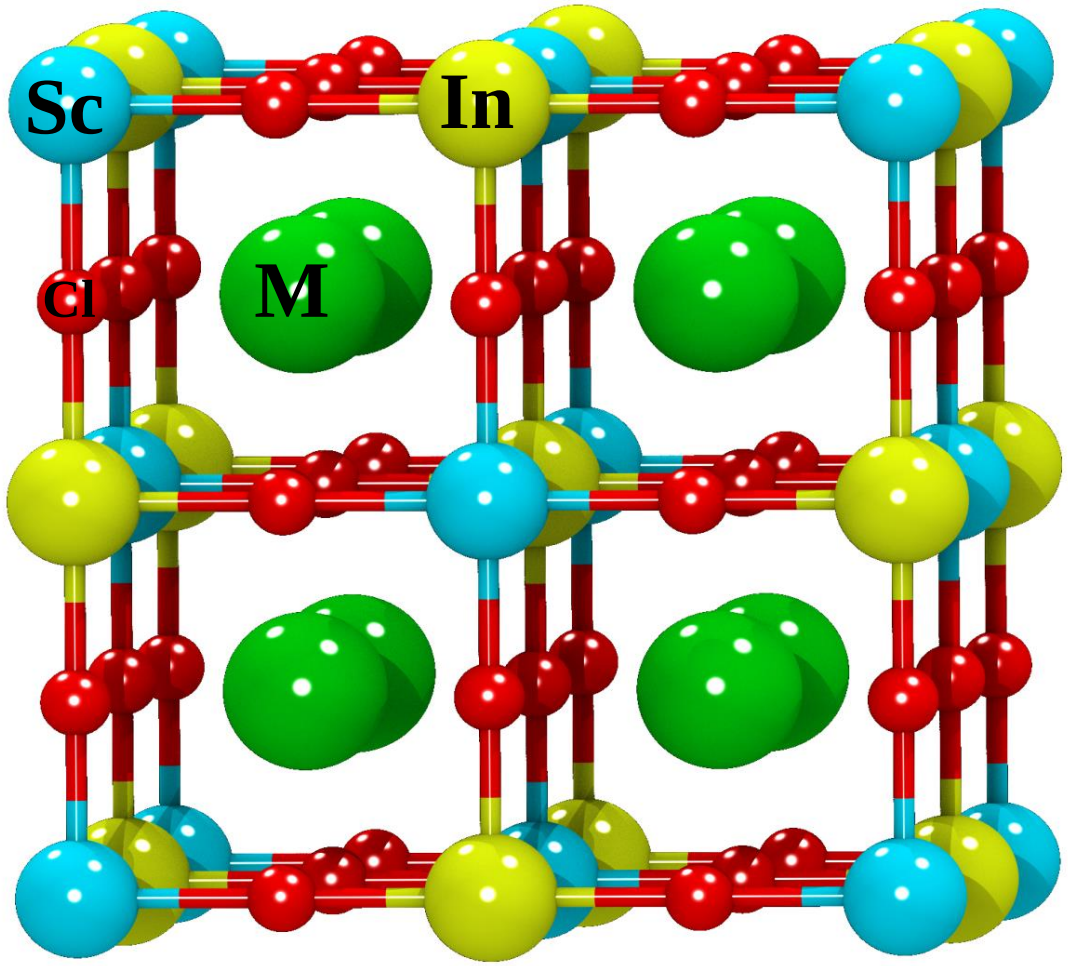
Lead-free double perovskites: $A_2B^+B^{3+}X_6$



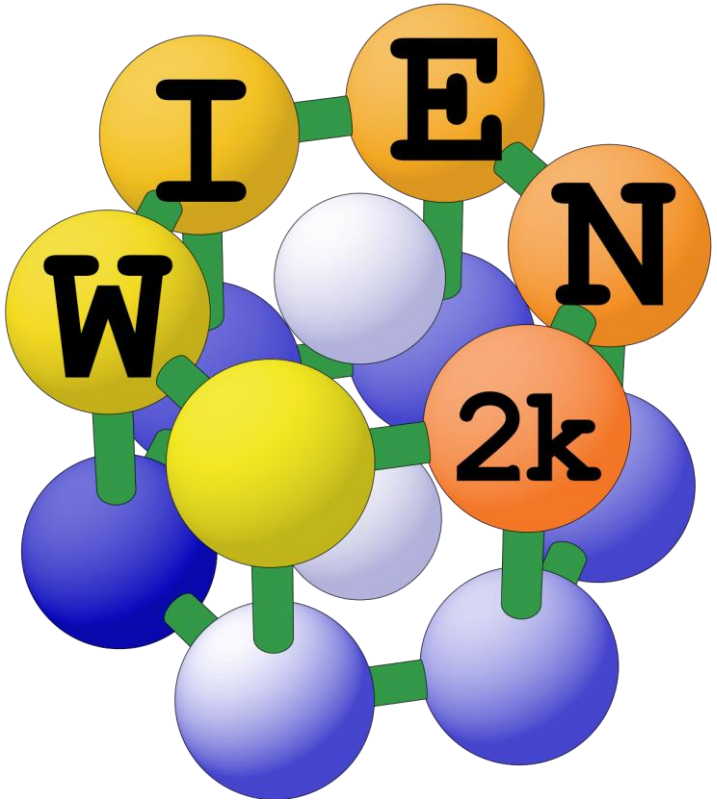
https://pubs.acs.org/doi/10.1021/acsenergylett.6b00499

Structure of $M_2ScInCl_6$ (M = Rb, Cs)



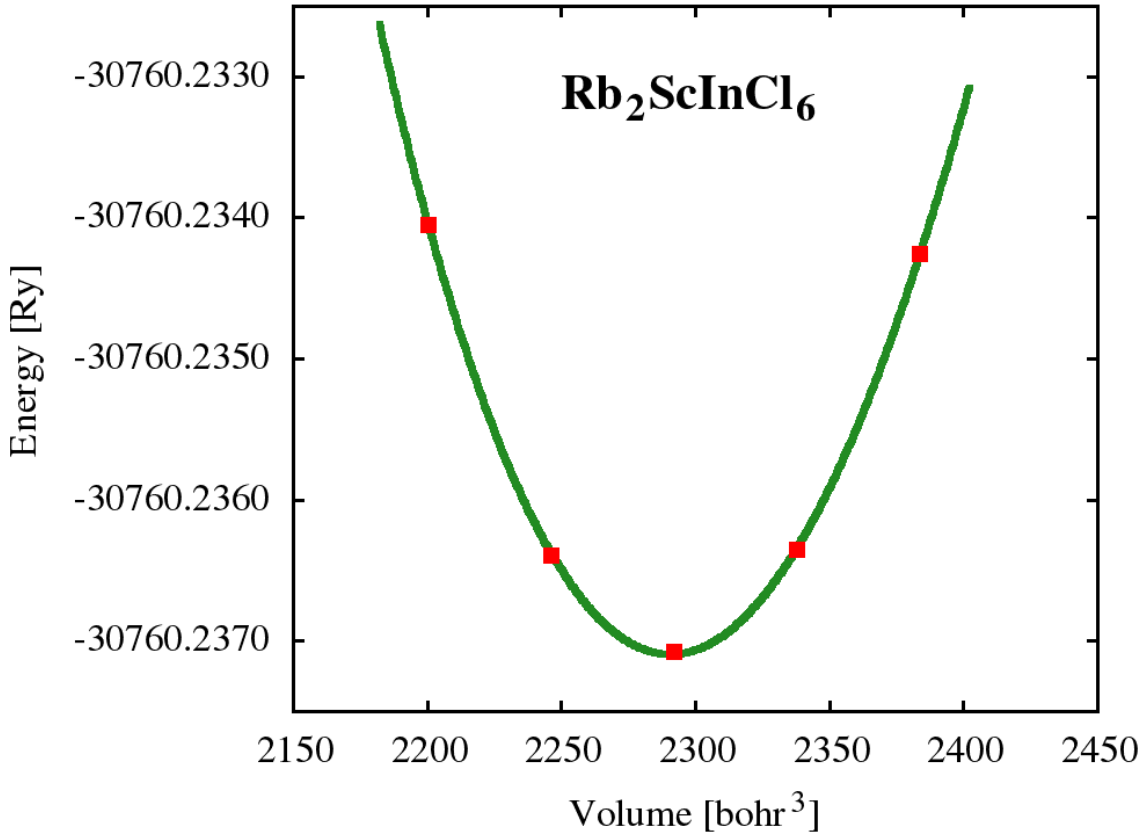


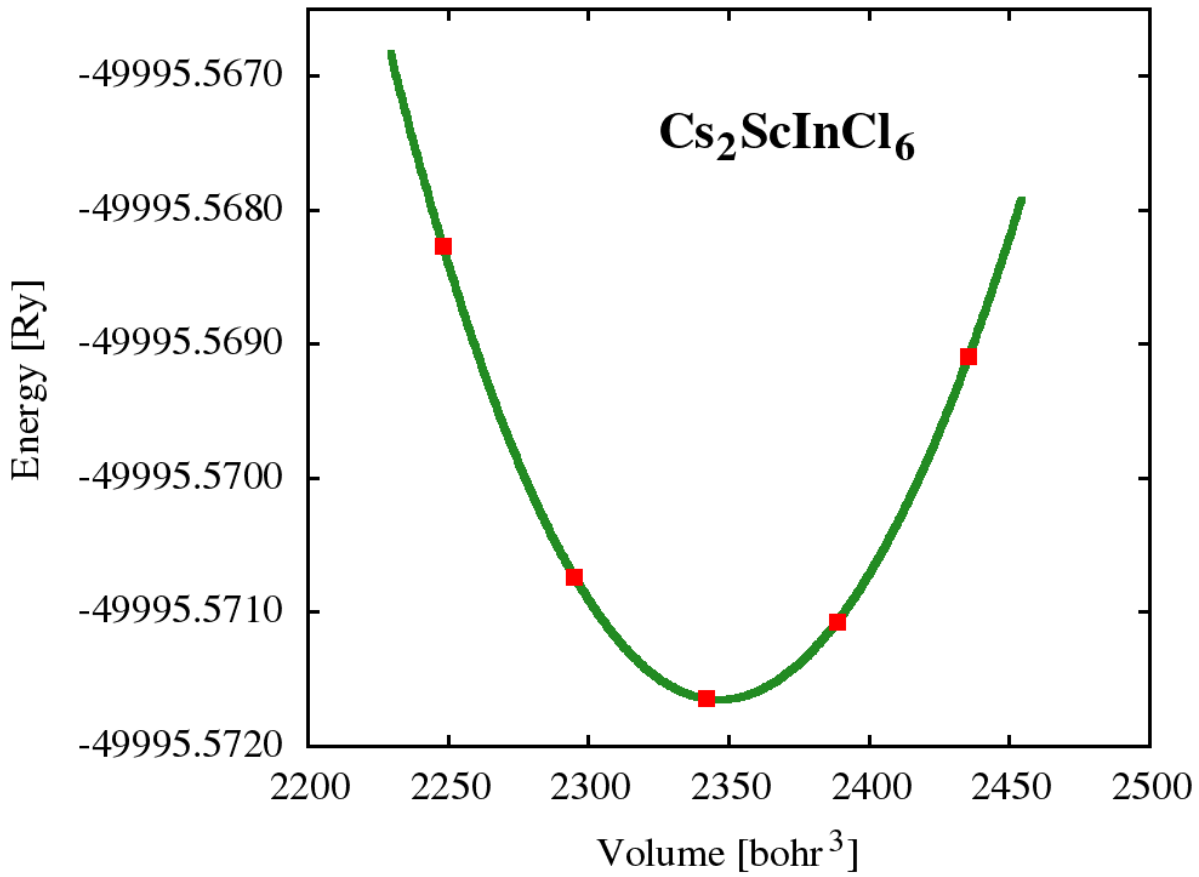
Computational details



- R_{MT}(Cs, In) = 2.50 a.u.
- R_{MT} (Rb, Sc) = 2.35 a.u.
- R_{MT} (Cl) = 1.15 a.u.
- $R_{MT} \times K_{max}$ = 8.0
- K-mesh = 10×10×10
- EC = 0.00001 Ry & CC = 0.0001 *e*

Optimized Lattice parameters

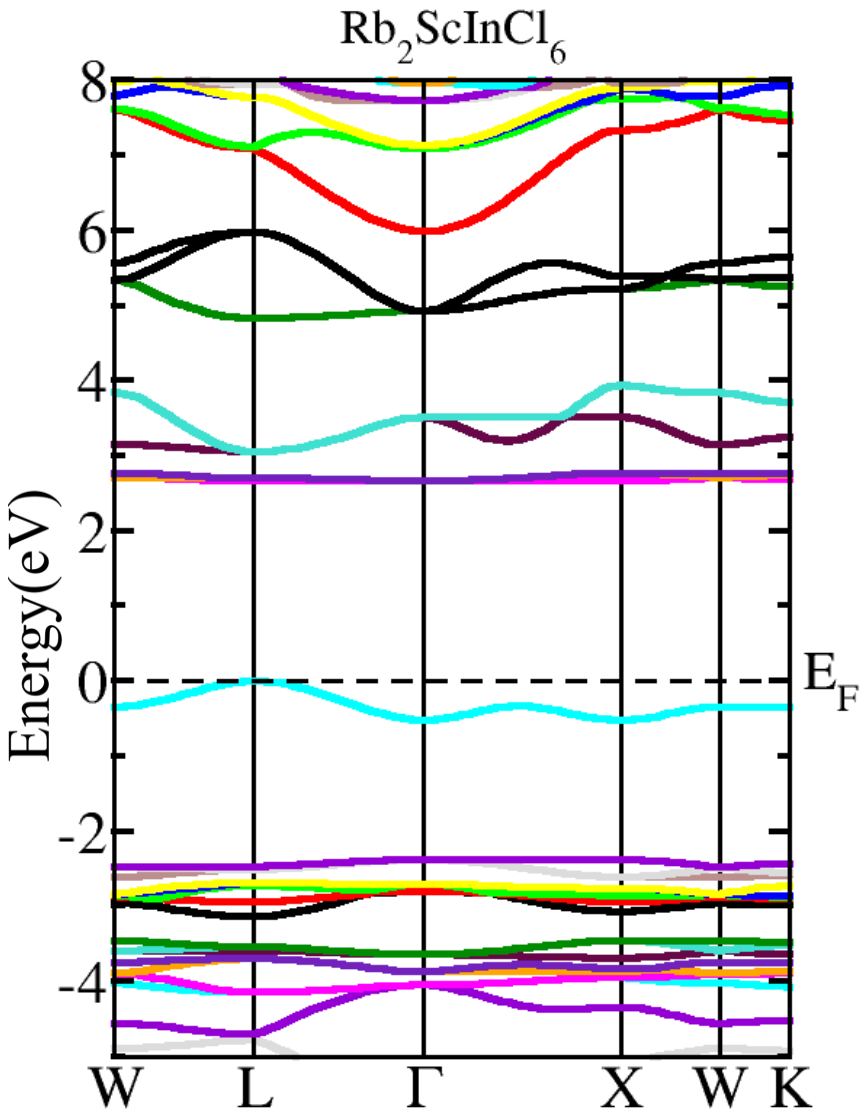


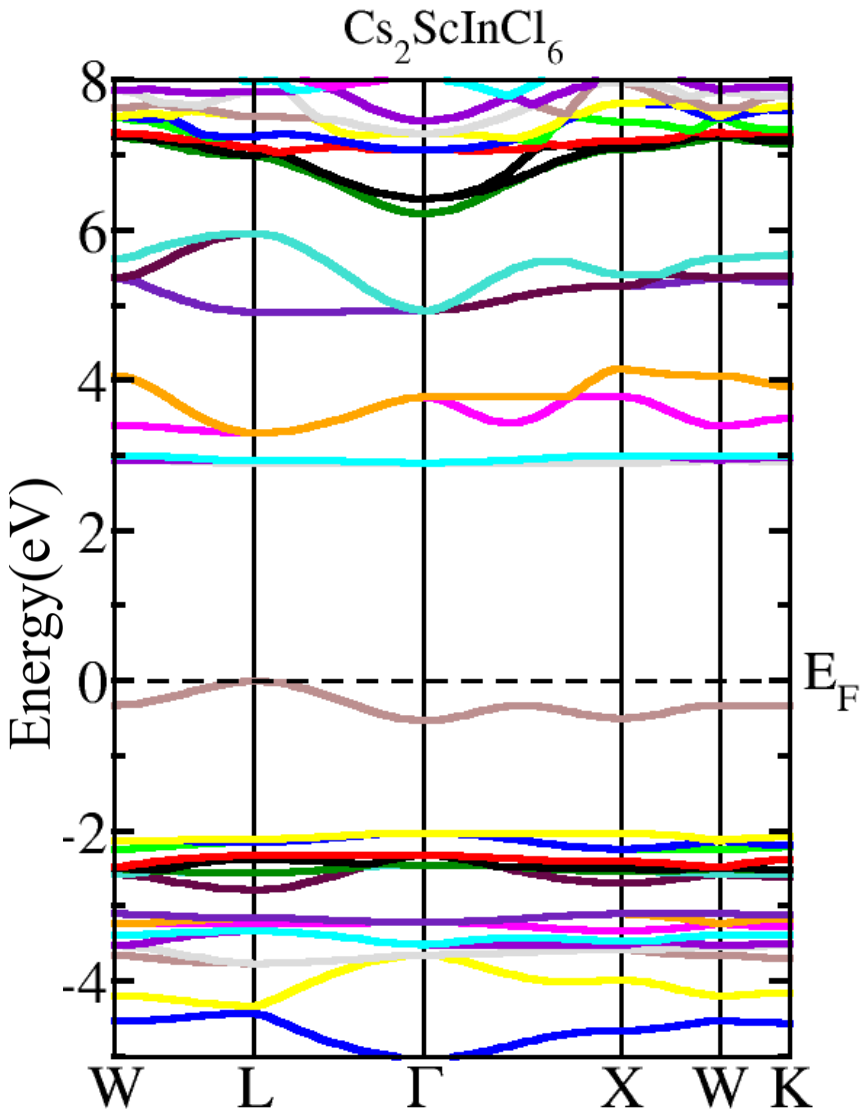


Optimized Lattice parameters

System	Lattice parameter (Å)	Band gap (eV)	
		PBE-GGA	TB-mBJ
$Rb_2ScInCl_6$	11.073	2.599	2.662
$Cs_2ScInCl_6$	11.163	2.802	2.902

Electronic properties





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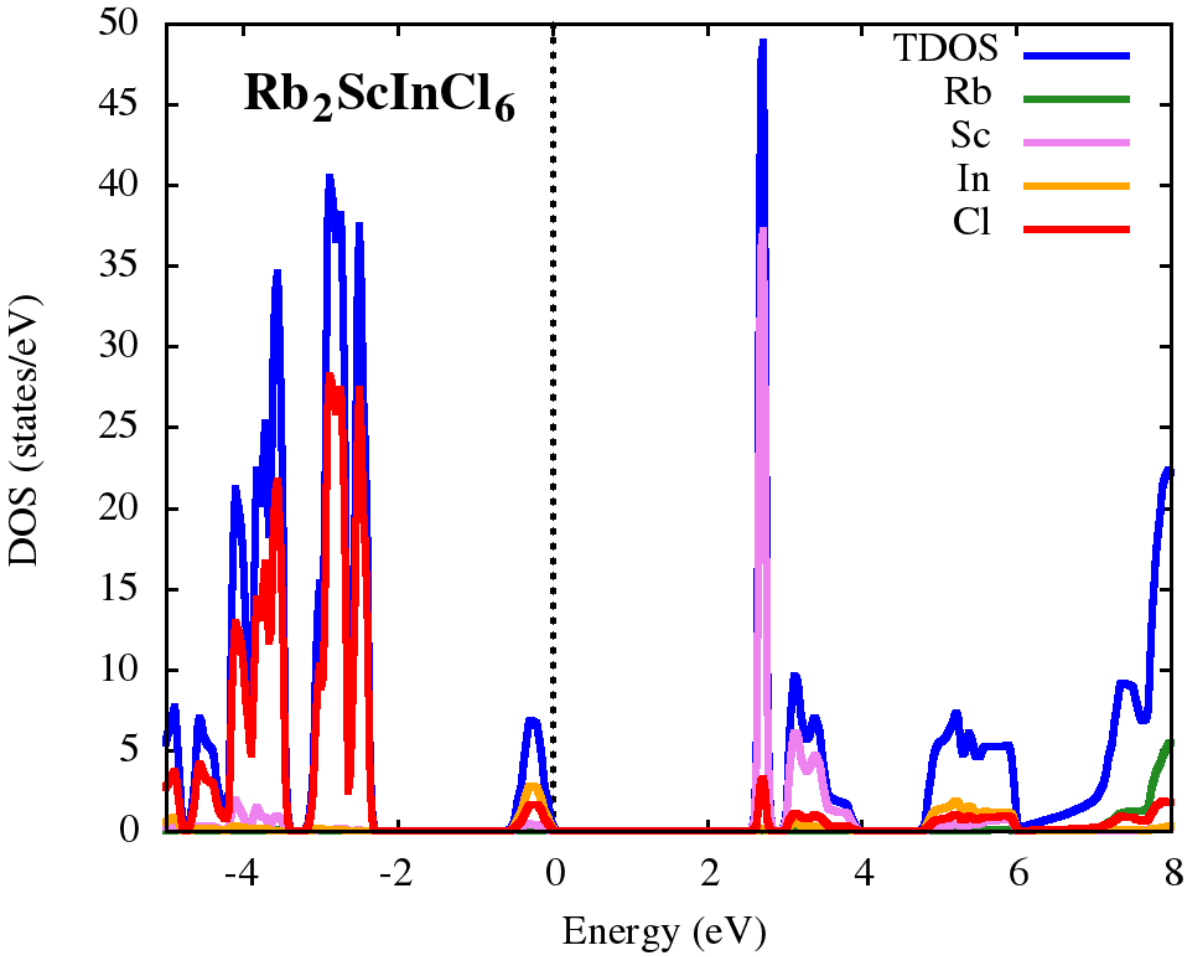
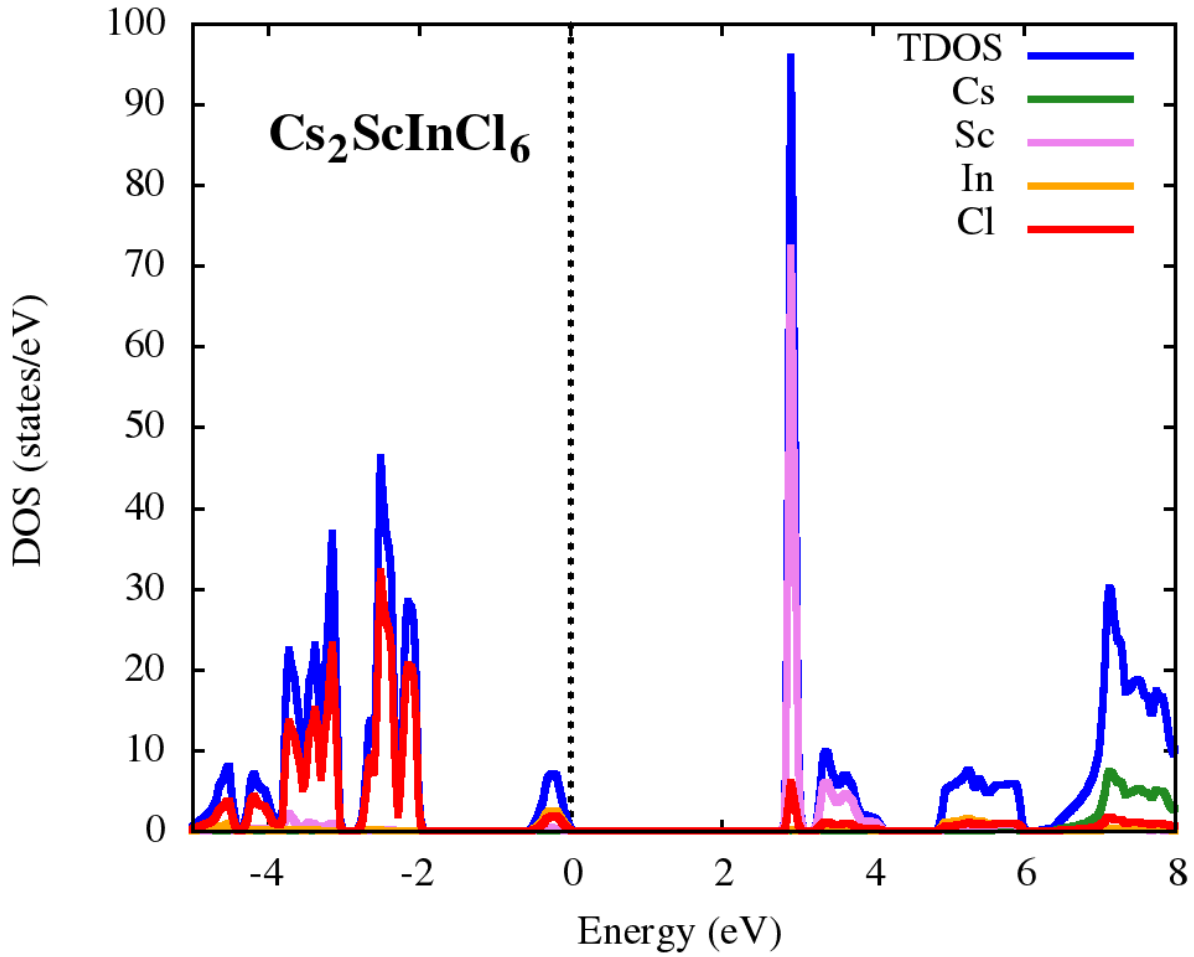
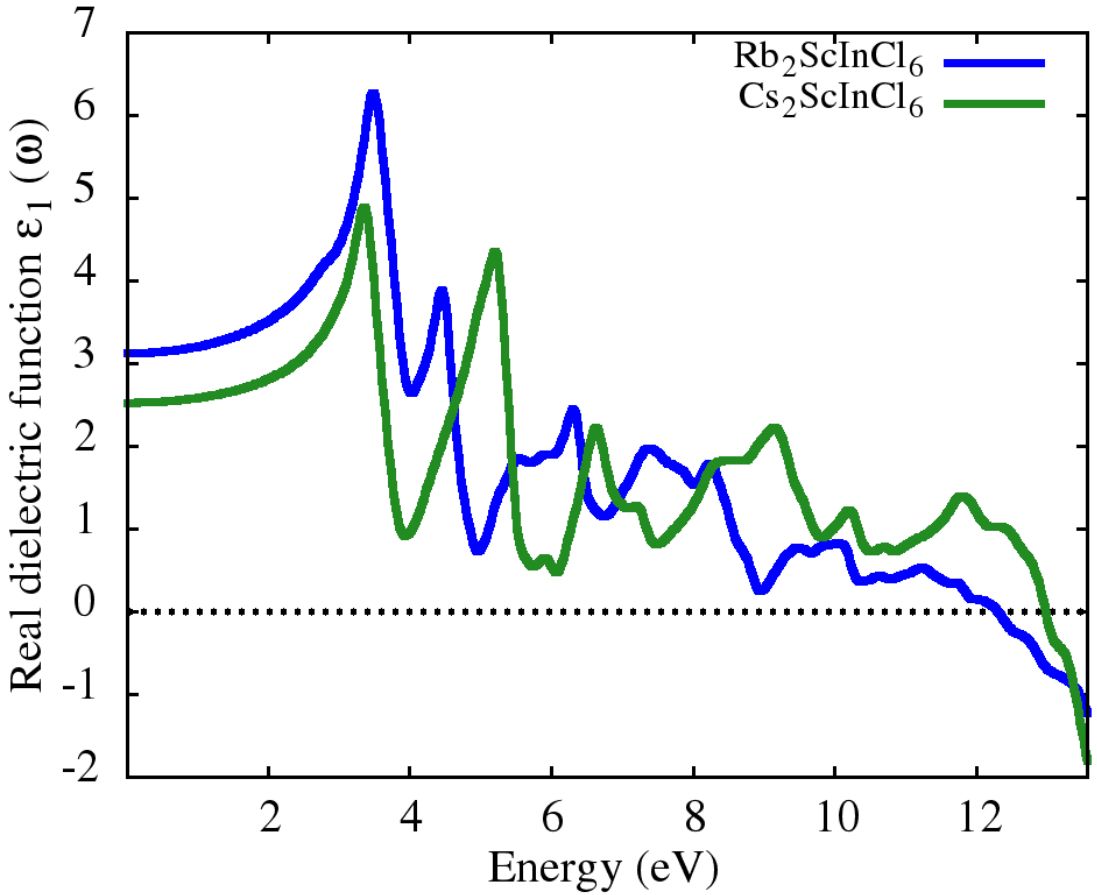
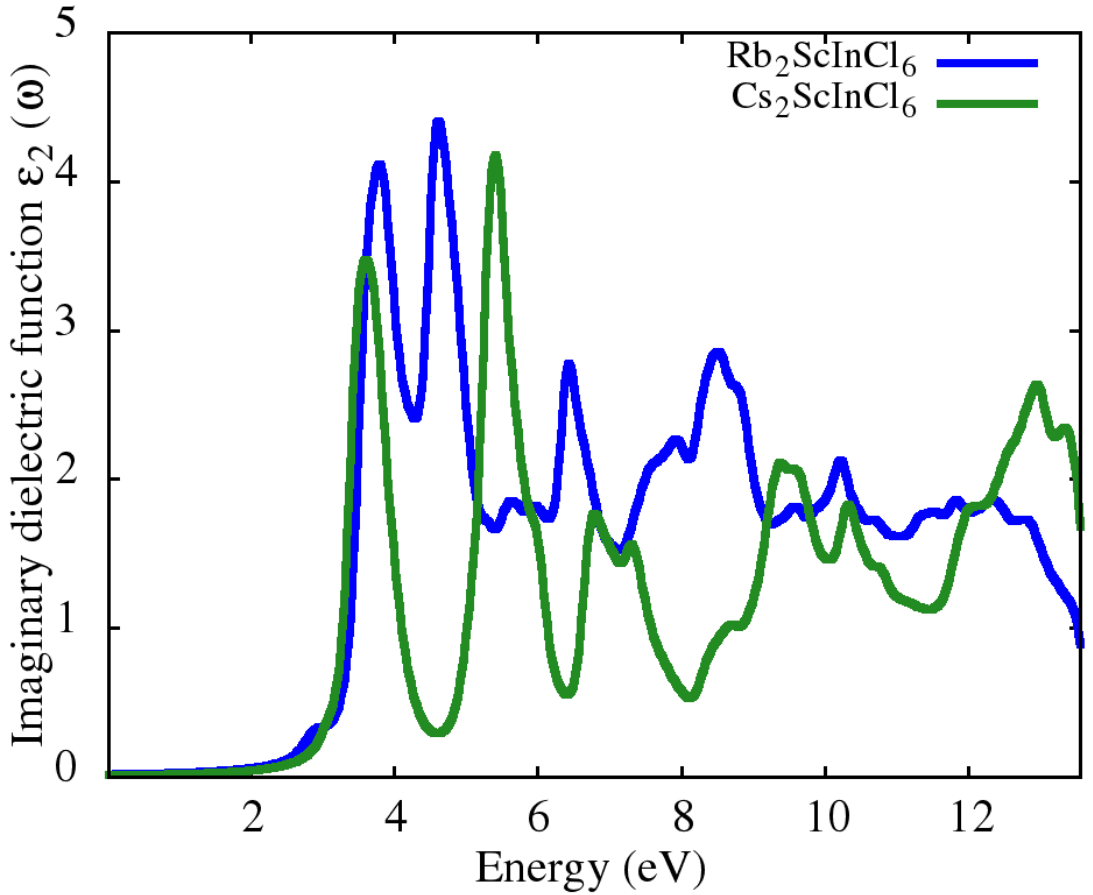




Optical properties

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$





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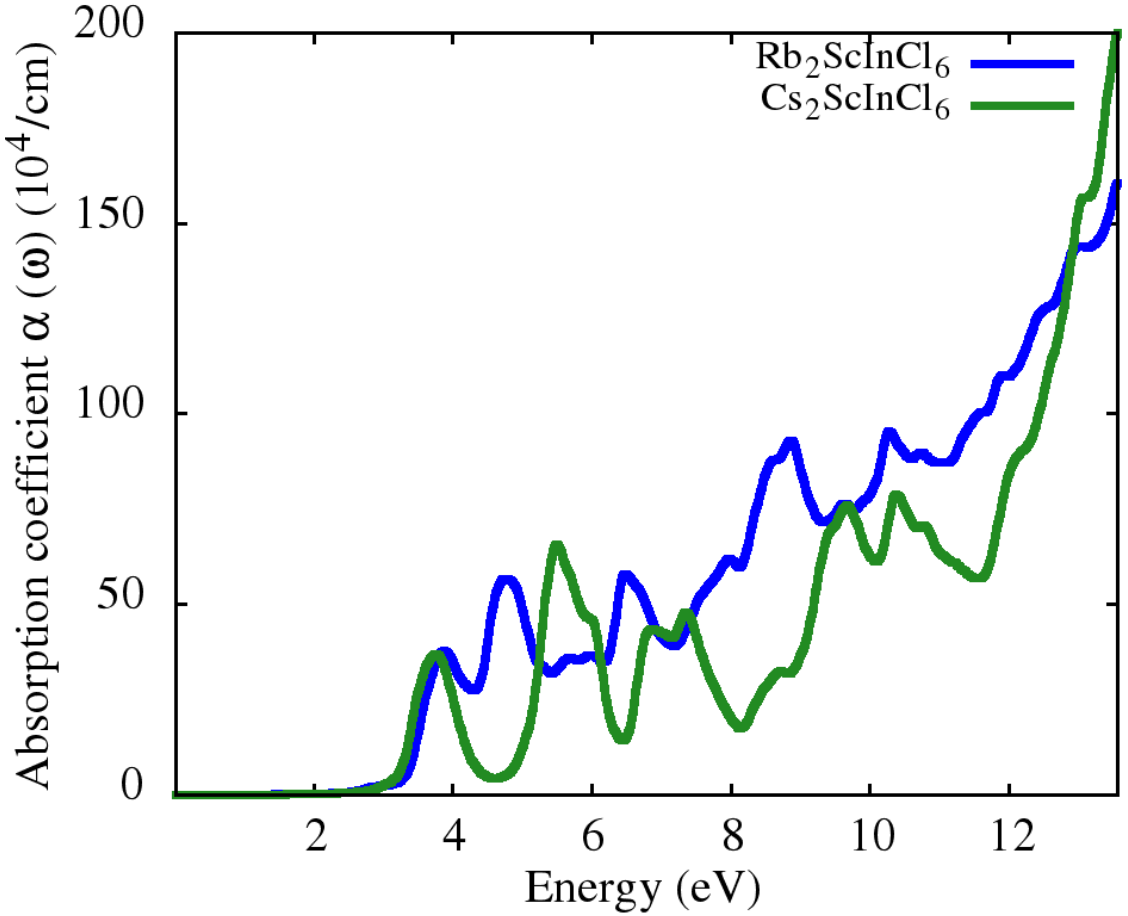

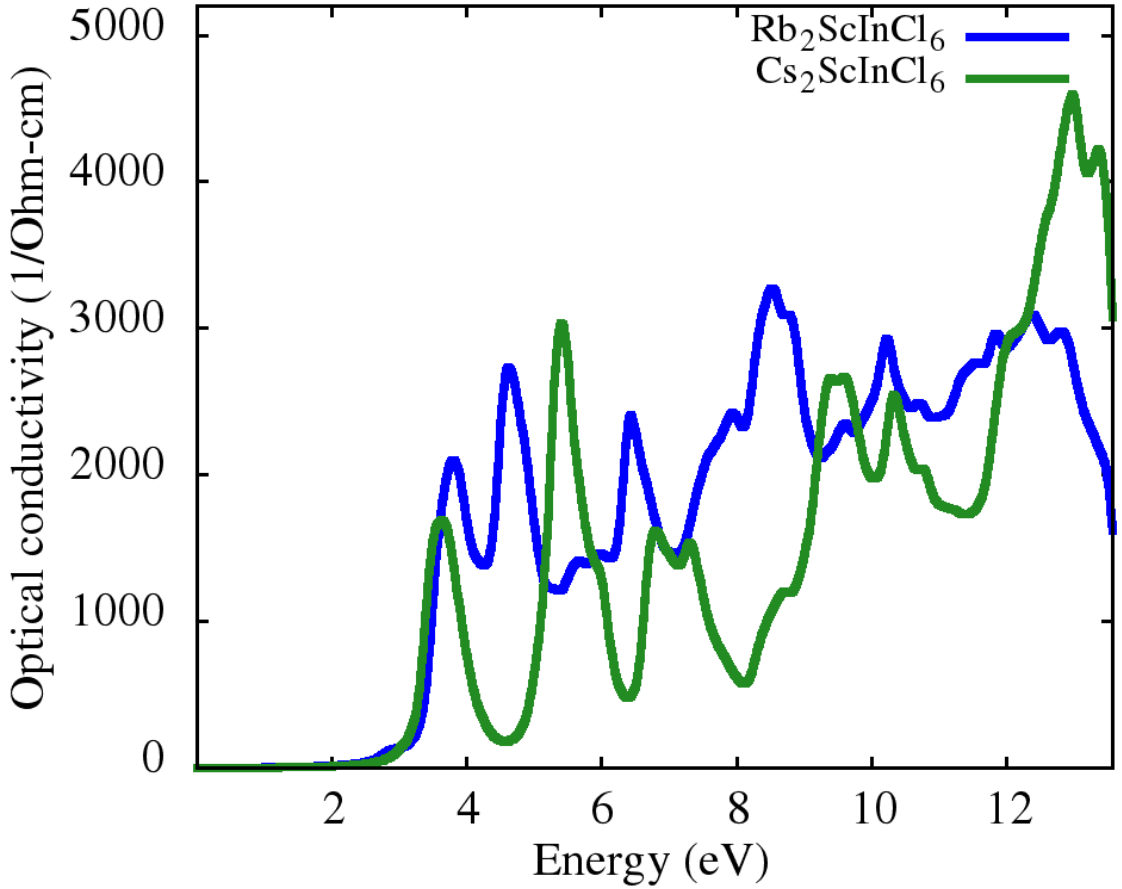

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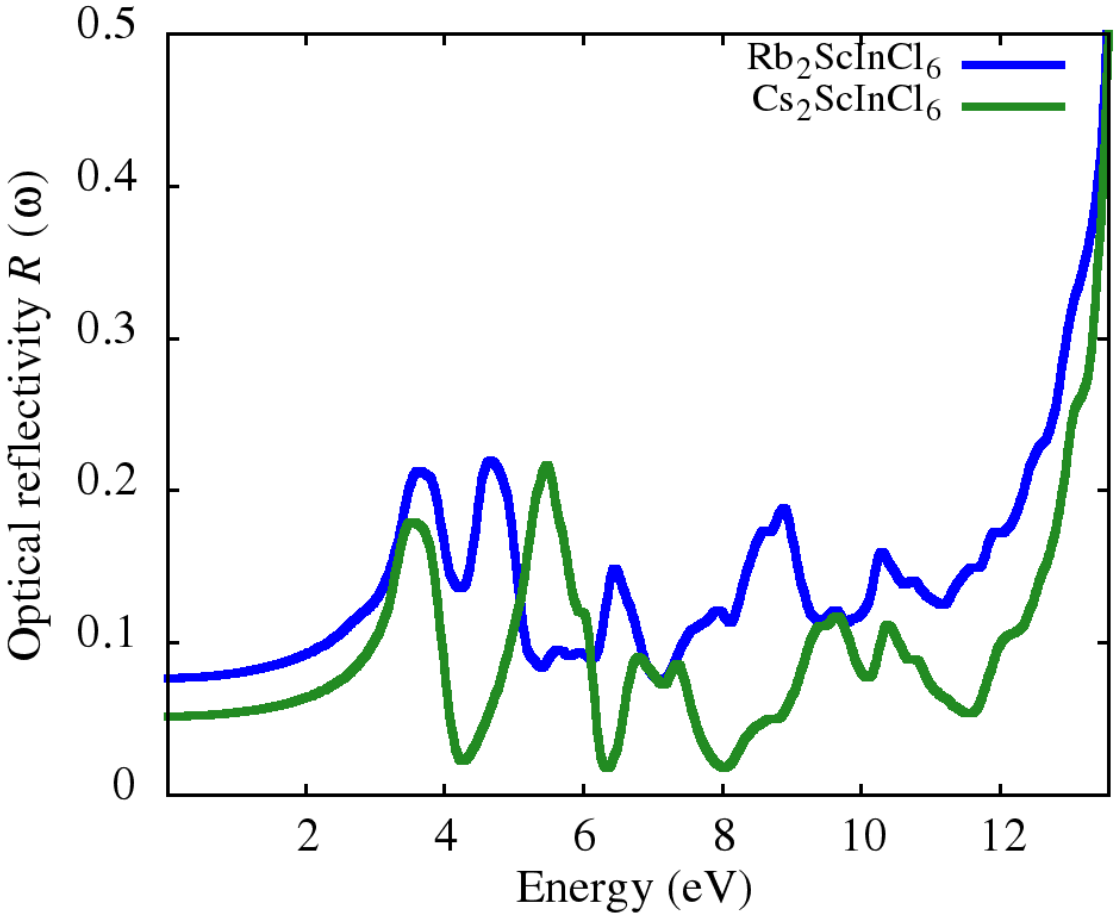
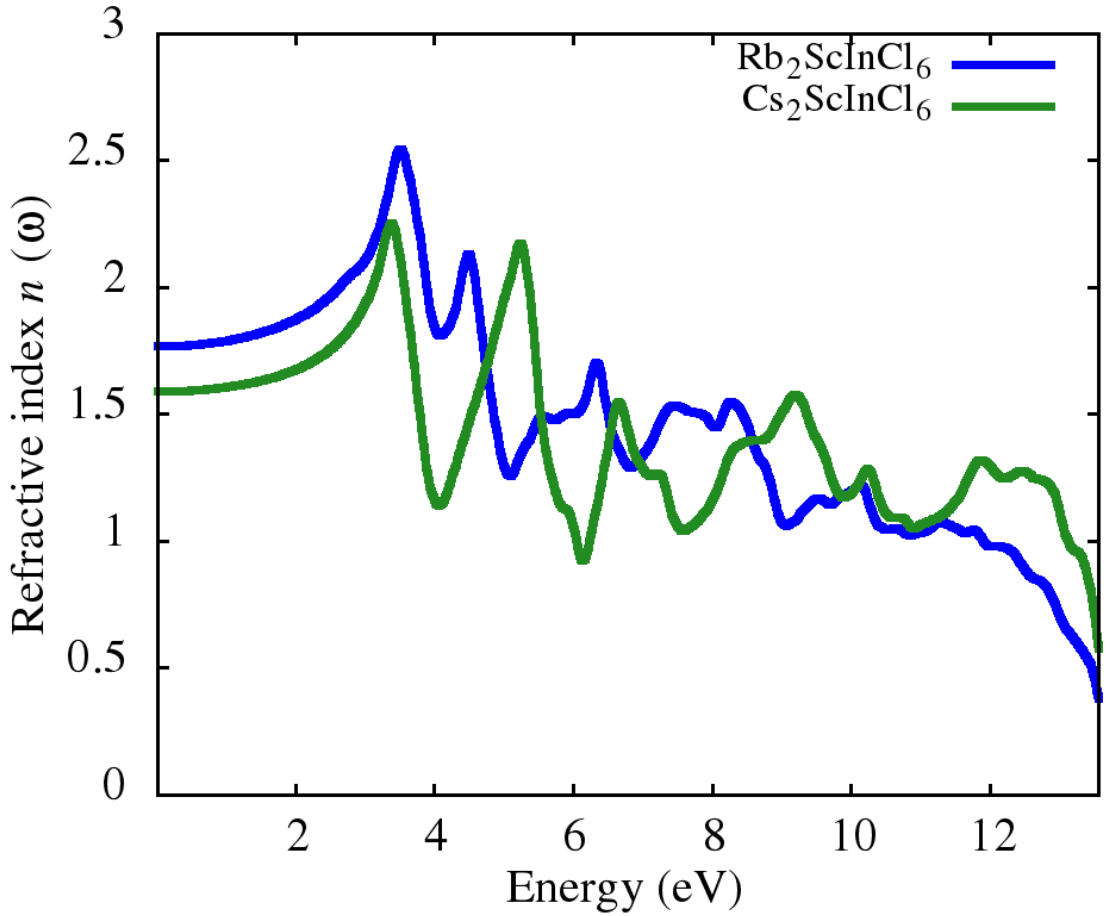
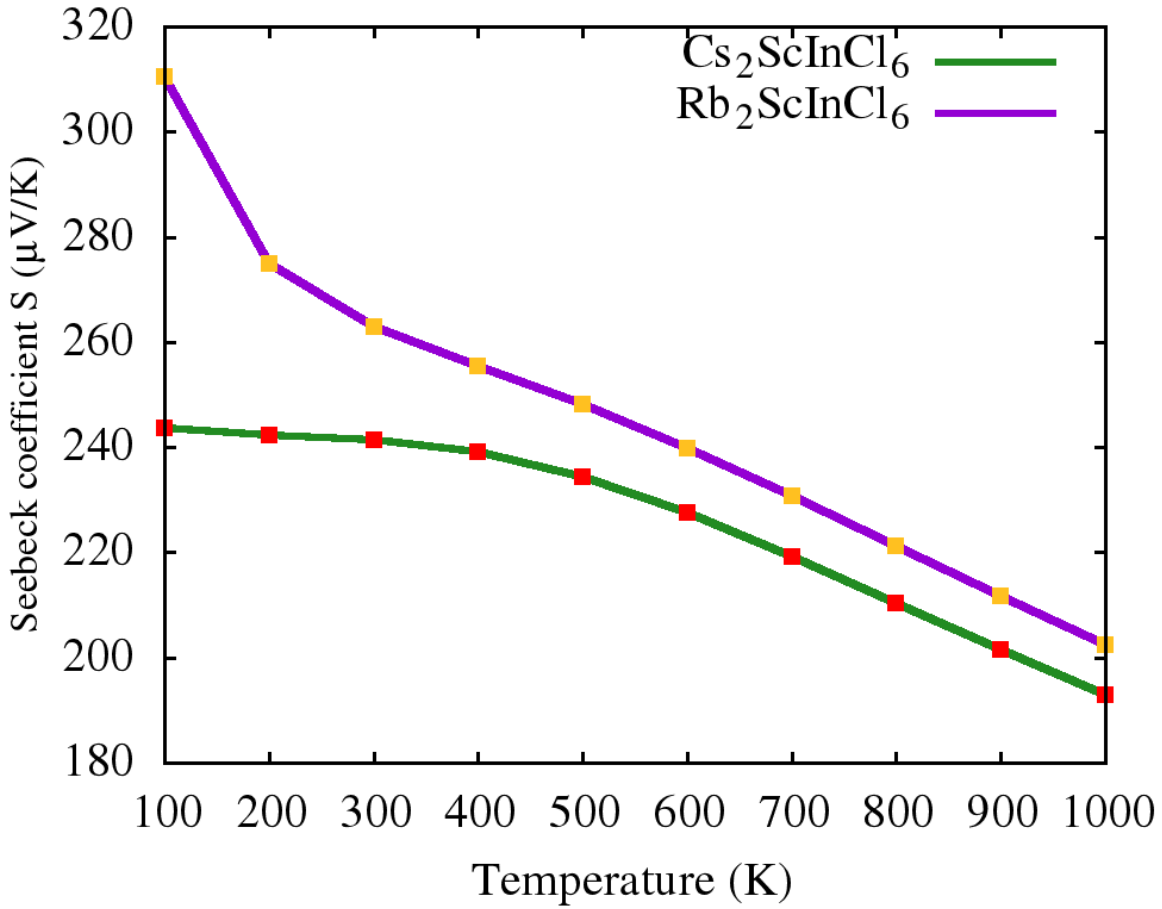
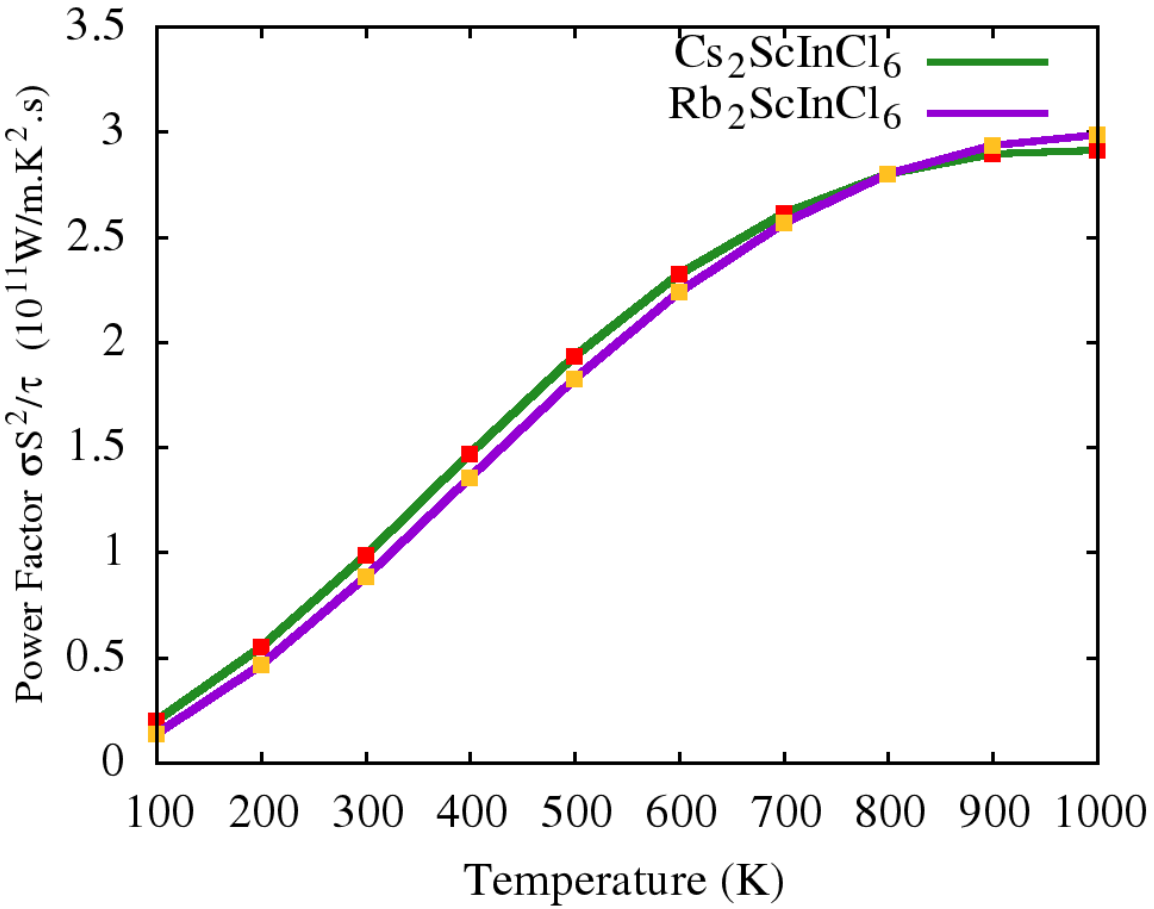


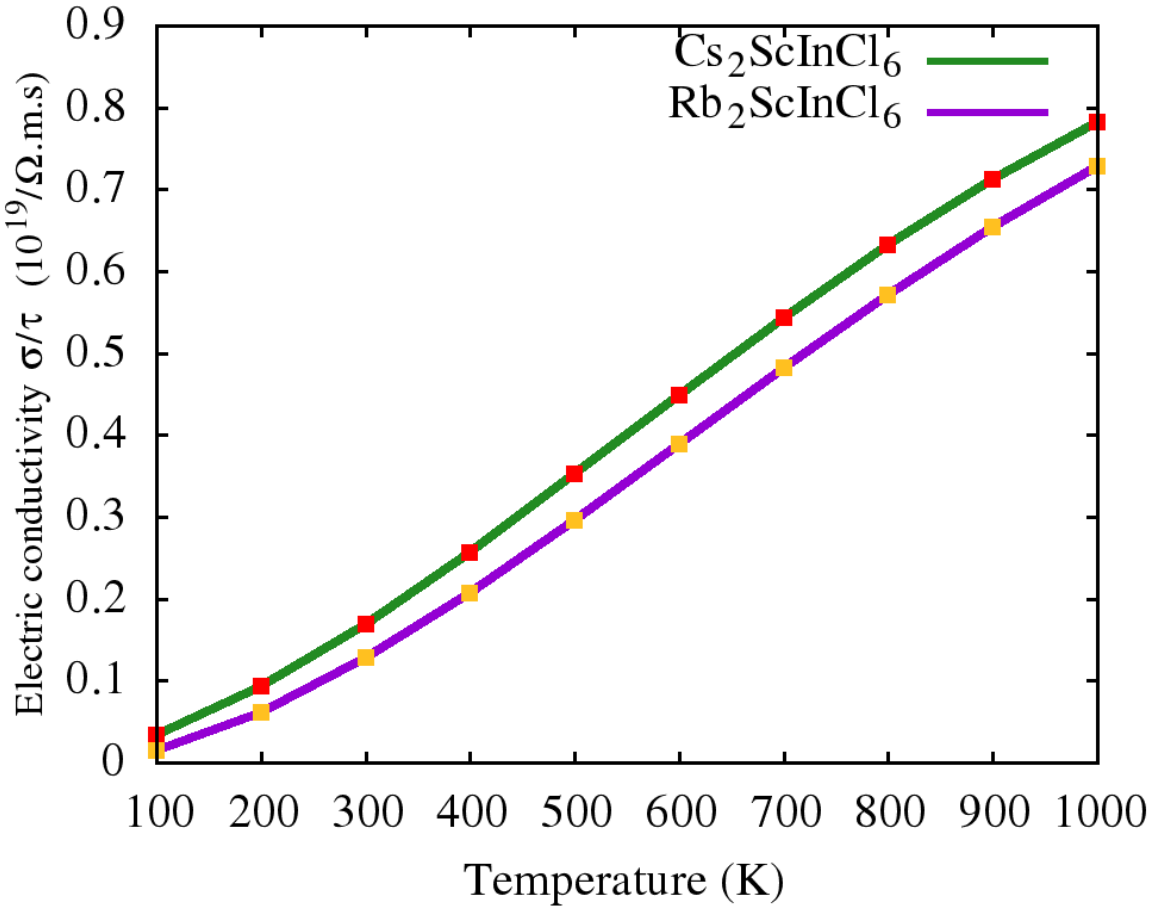


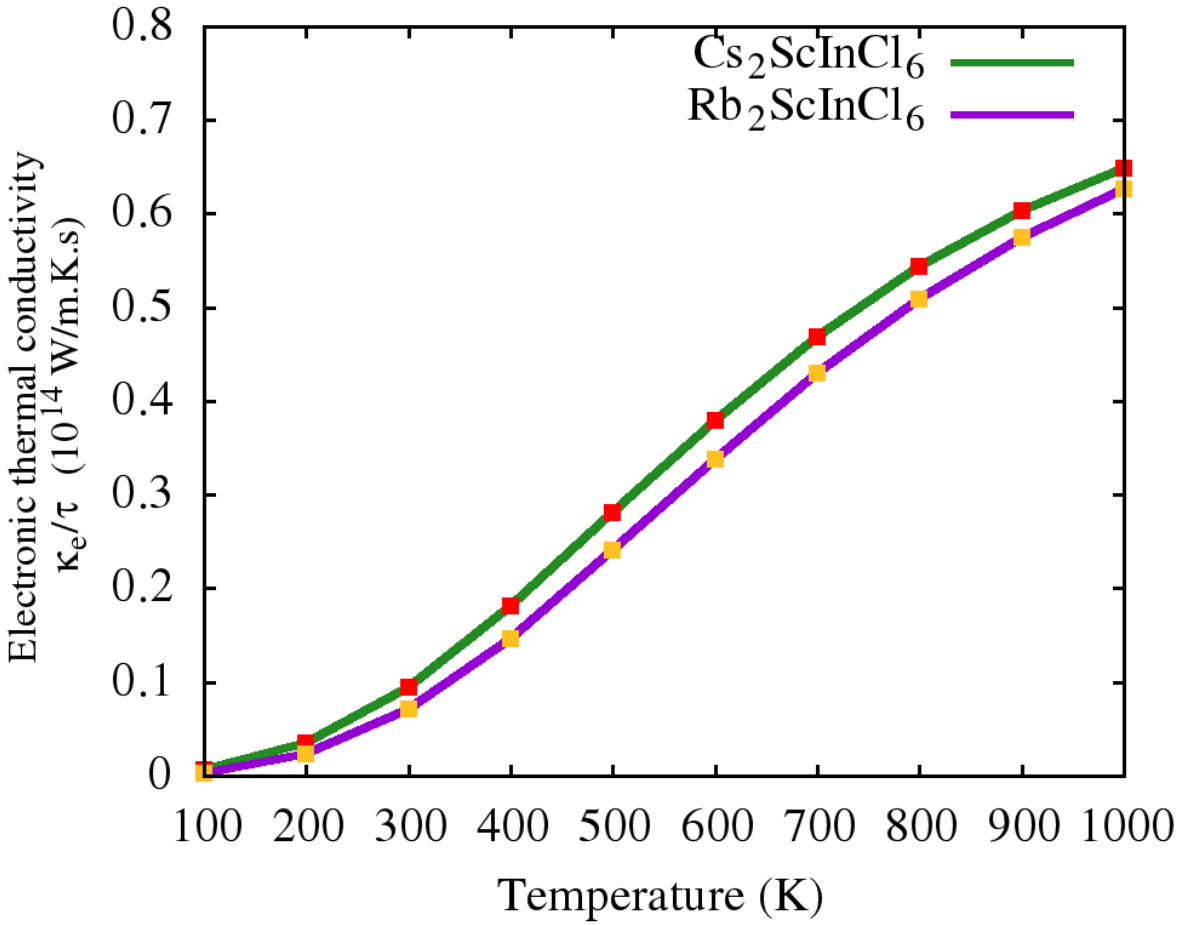
Thermoelectric properties





Thermoelectric properties





Conclusions

- Opto-electronic and thermoelectric properties double perovskites $M_2ScInCl_6$ (M=Rb, Cs) using WIEN2k
- Both compounds show semiconductor like behavior
- Remarkable optical properties
- Good Seebeck coefficient and power factor
- Promising materials for different opto-electronic and thermoelectric applications


“Thank you”