

First-principles calculations of opto-electronic and thermoelectric properties double perovskite semiconductors $M_2\text{ScInCl}_6$ ($M = \text{Rb}, \text{Cs}$)

Mohammad Abdur Rashid

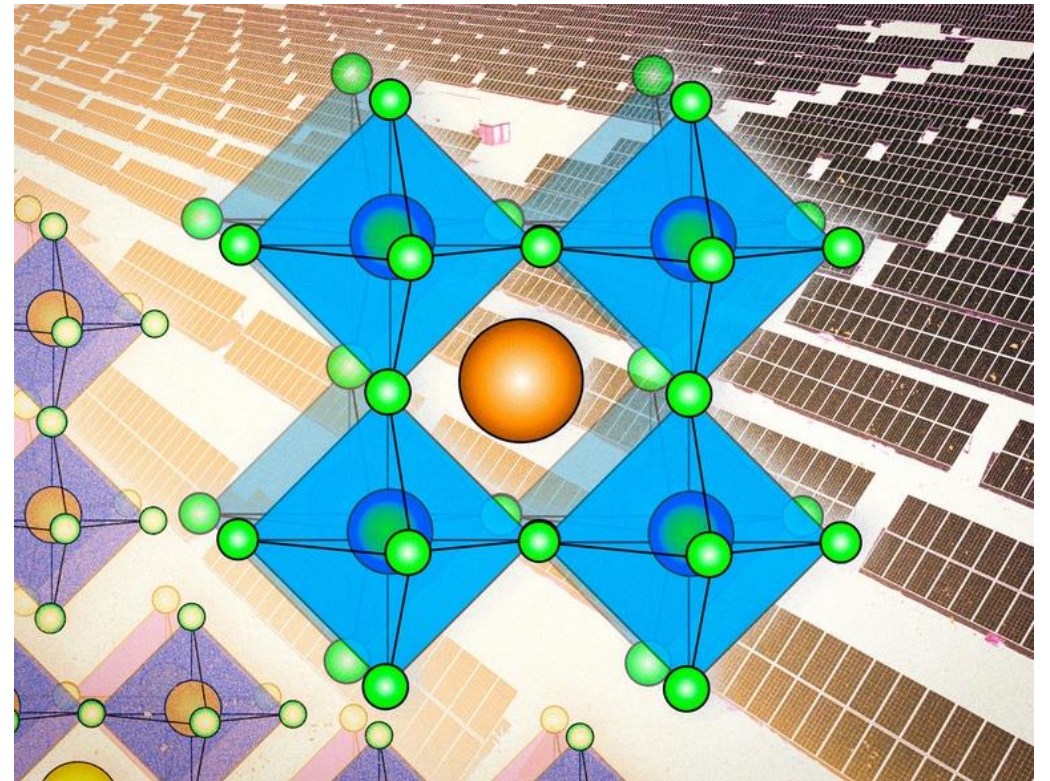
Md. Borhanul Asfia, Sahadat Jaman



Outline

- Lead-free double perovskite
- Our systems of study: $\text{Rb}_2\text{ScInCl}_6$ and $\text{Cs}_2\text{ScInCl}_6$
- Computational details
- Opto-electronic properties
- Thermoelectric properties
- Conclusions

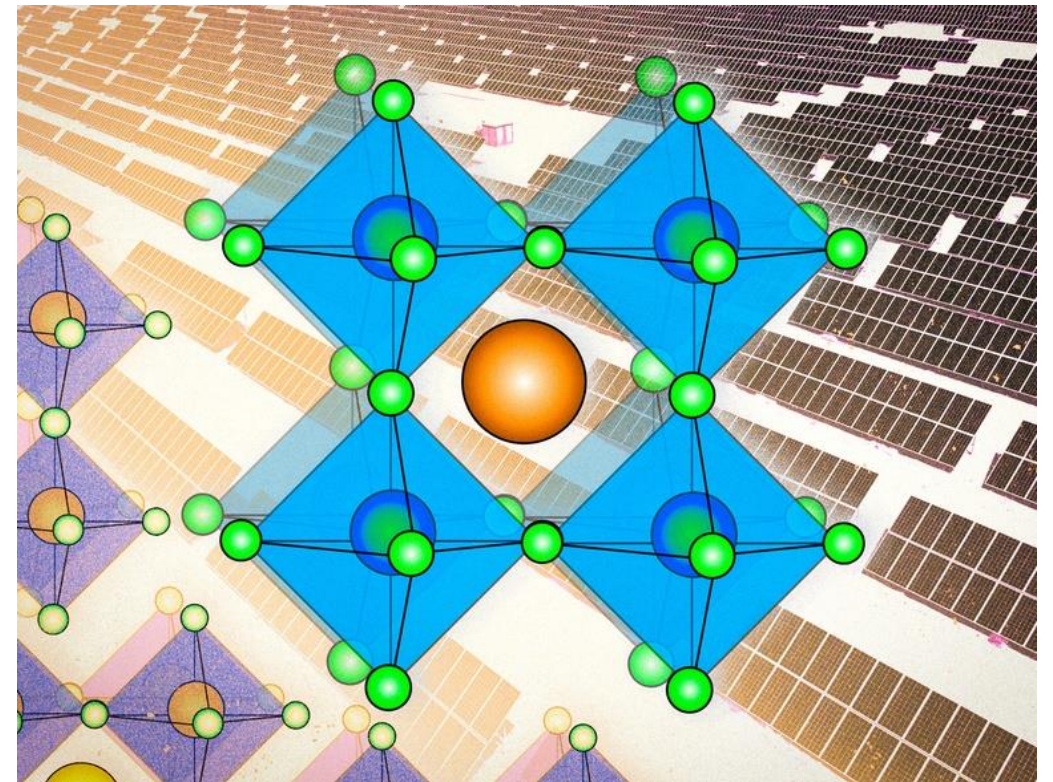
Perovskite solar cells



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

Perovskite solar cells

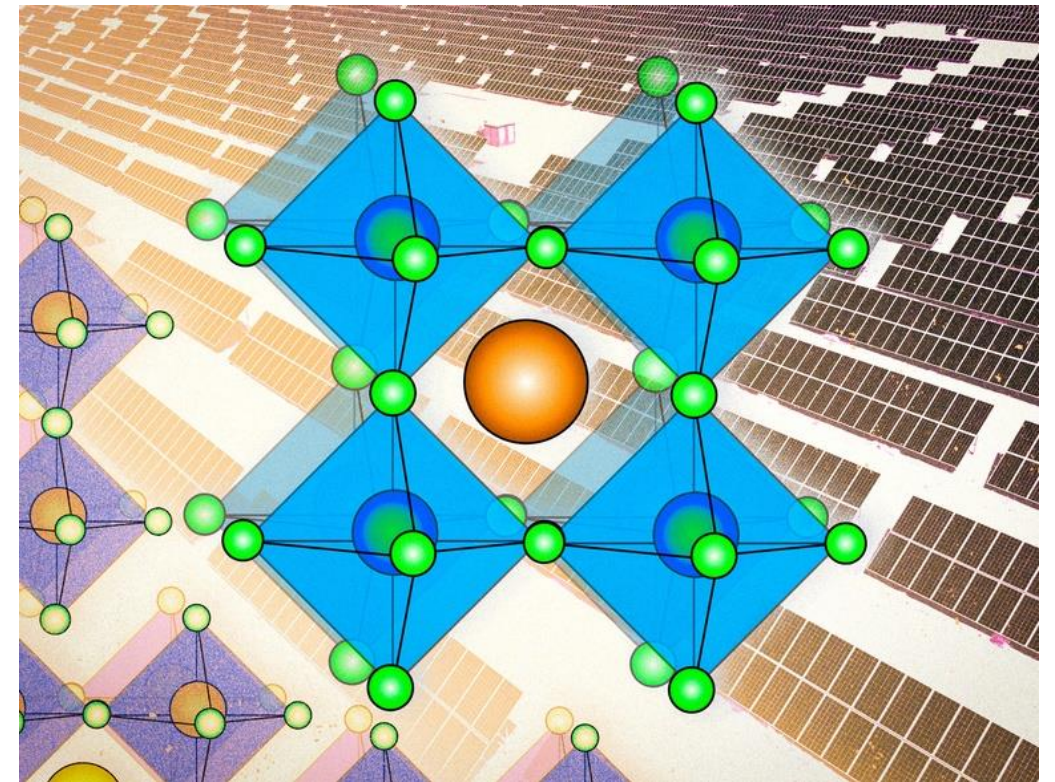
- High power conversion efficiency (about 25%)
- Easier manufacturing process
- Lower cost and greater flexibility



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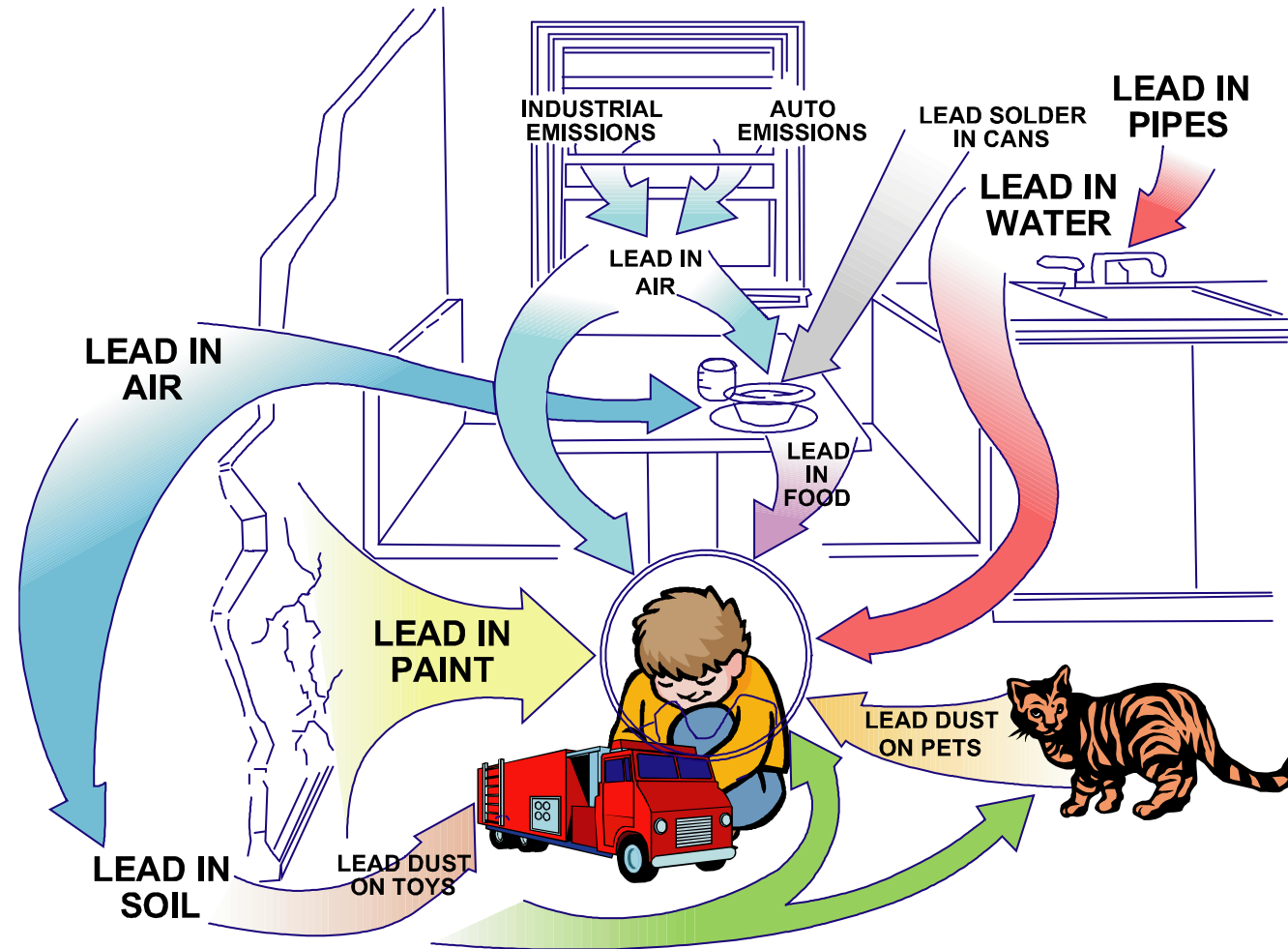
Perovskite solar cells

- 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



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

Environmental sources of lead exposure



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

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

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac															

57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

<div>NH₄⁺</div> <div>CH₃NH₃⁺</div>	<div>CN⁻</div>
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A₂

B

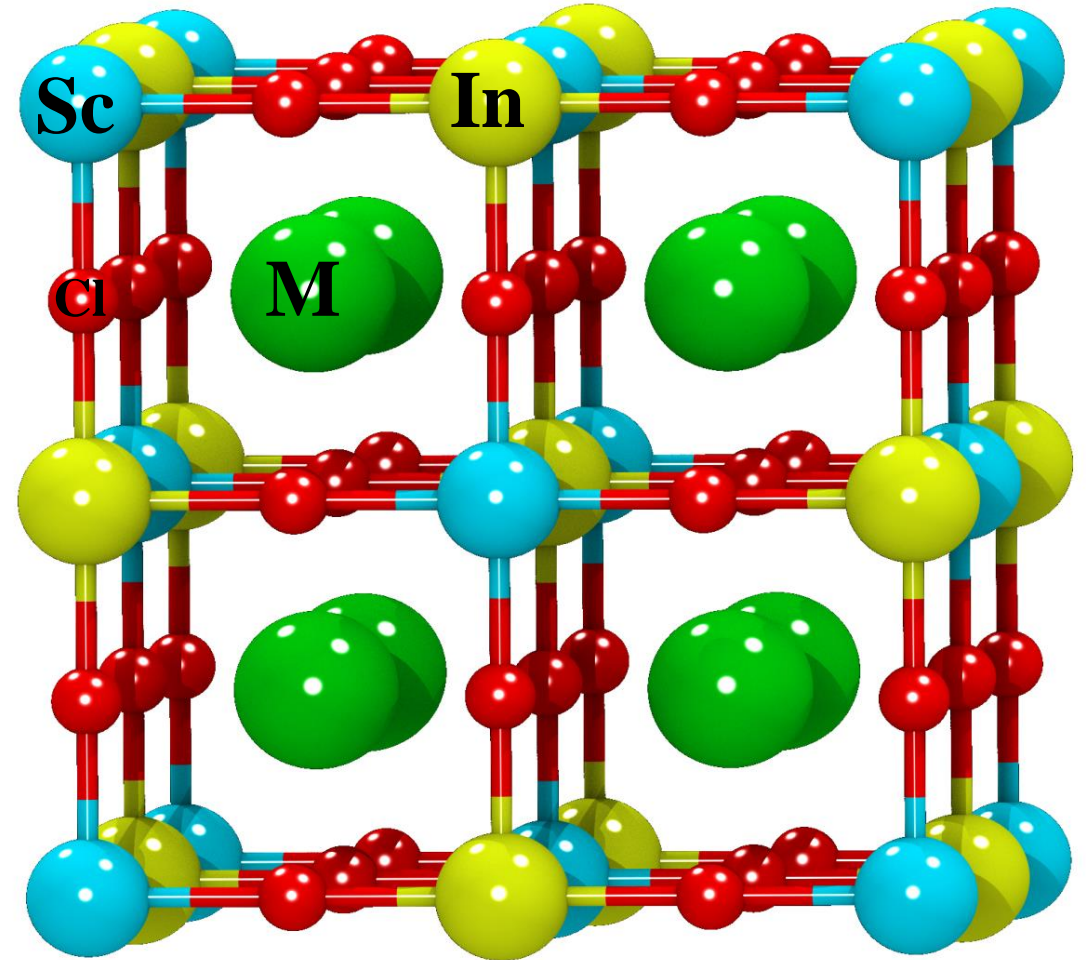
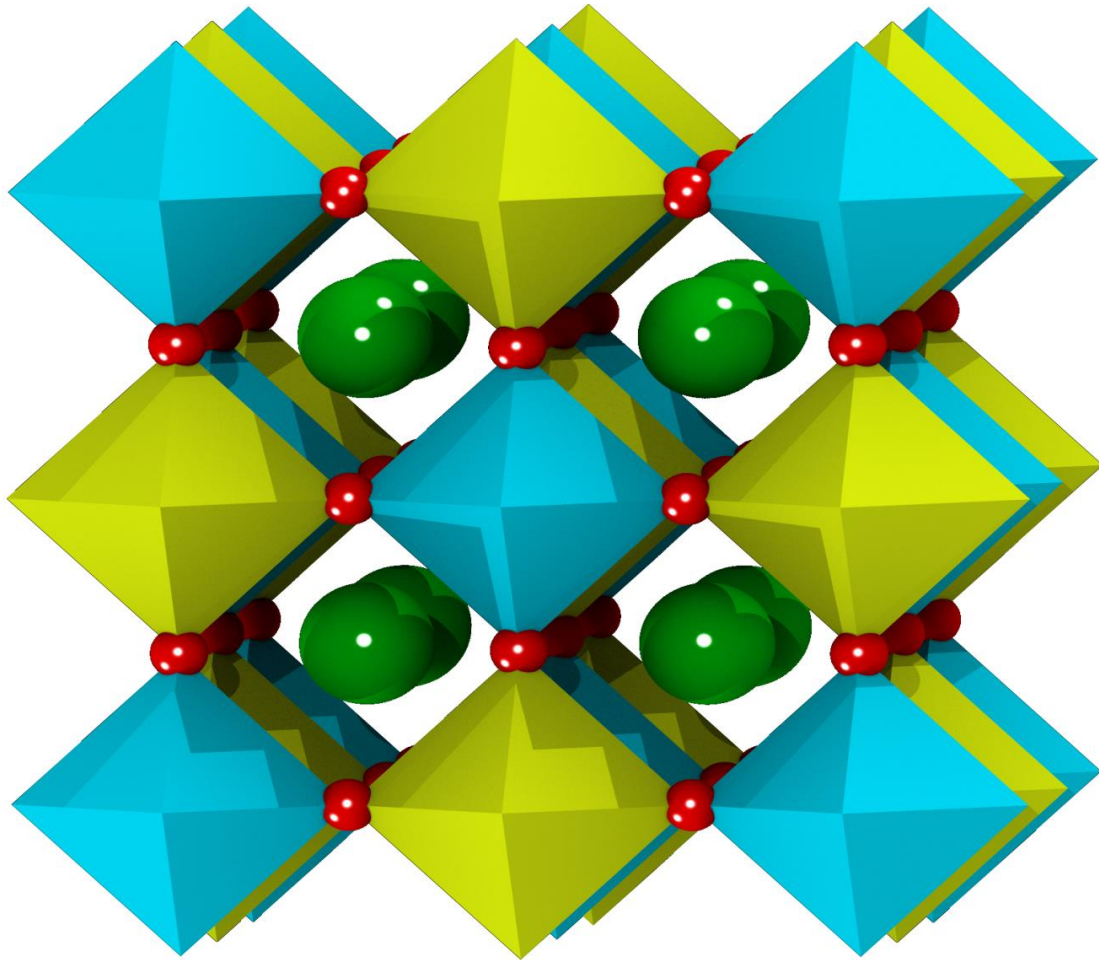
B³⁺

X₆

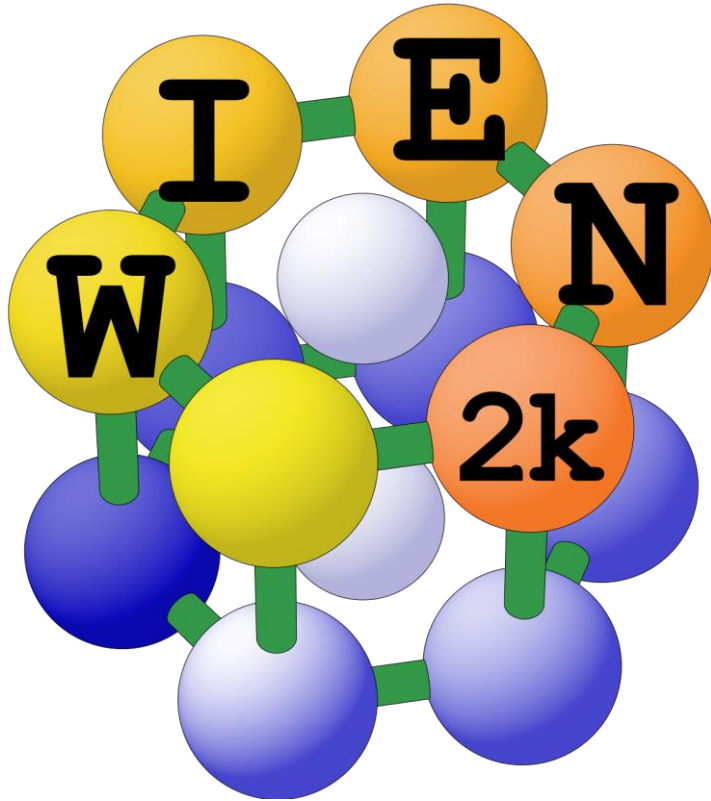
<https://pubs.acs.org/doi/10.1021/acseenergylett.6b00499>



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

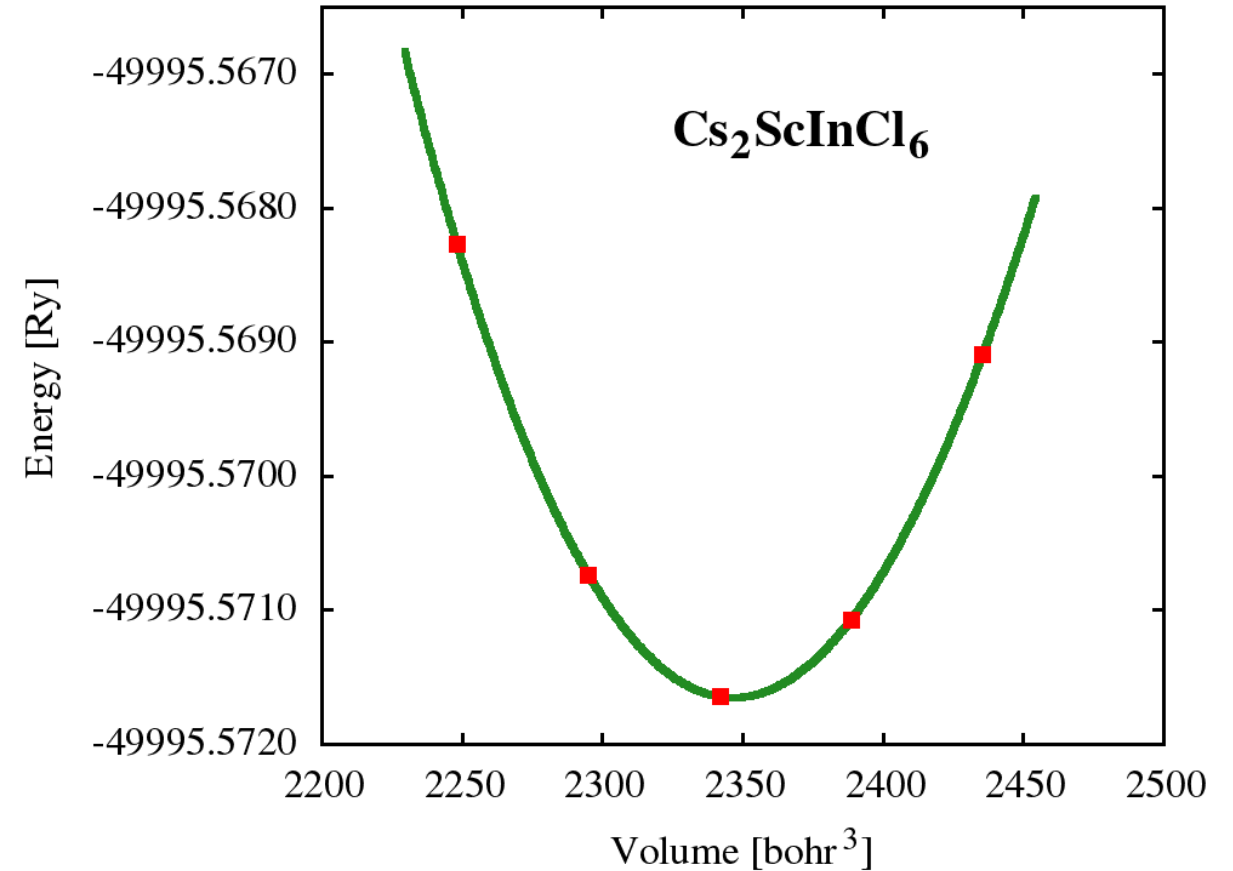
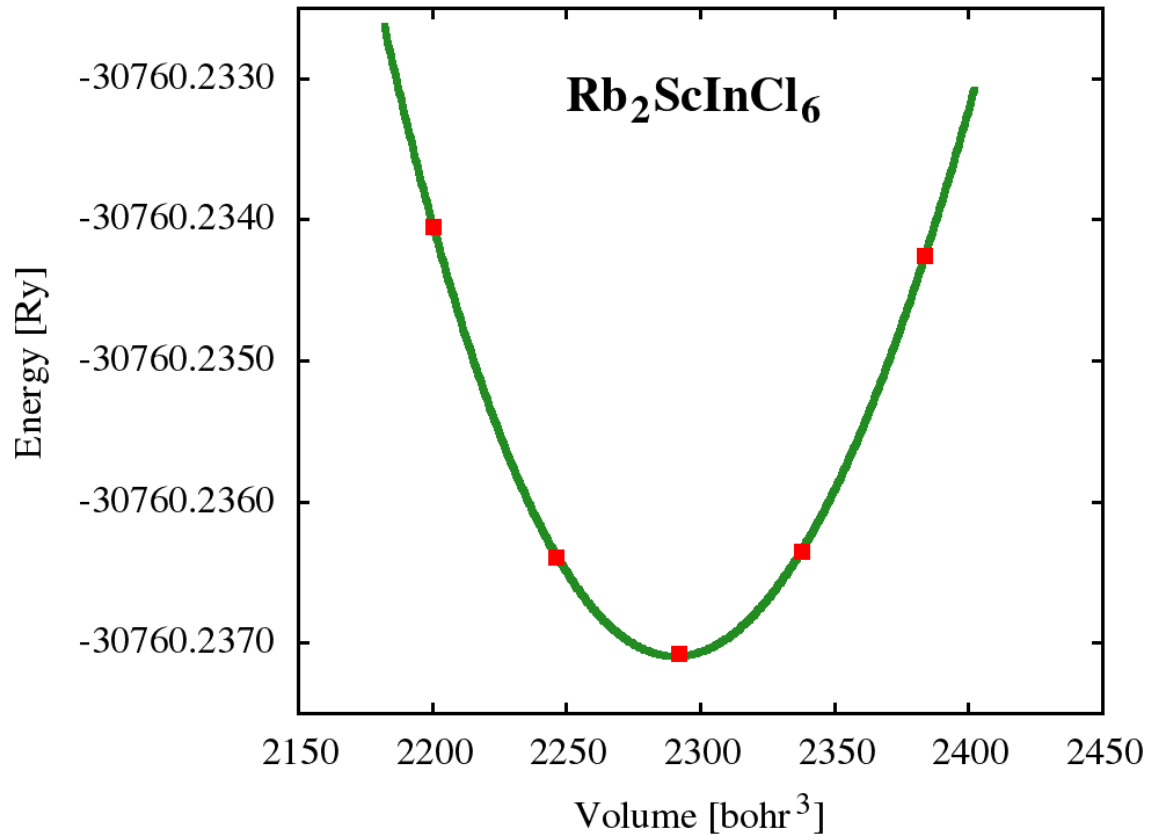


Computational details



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

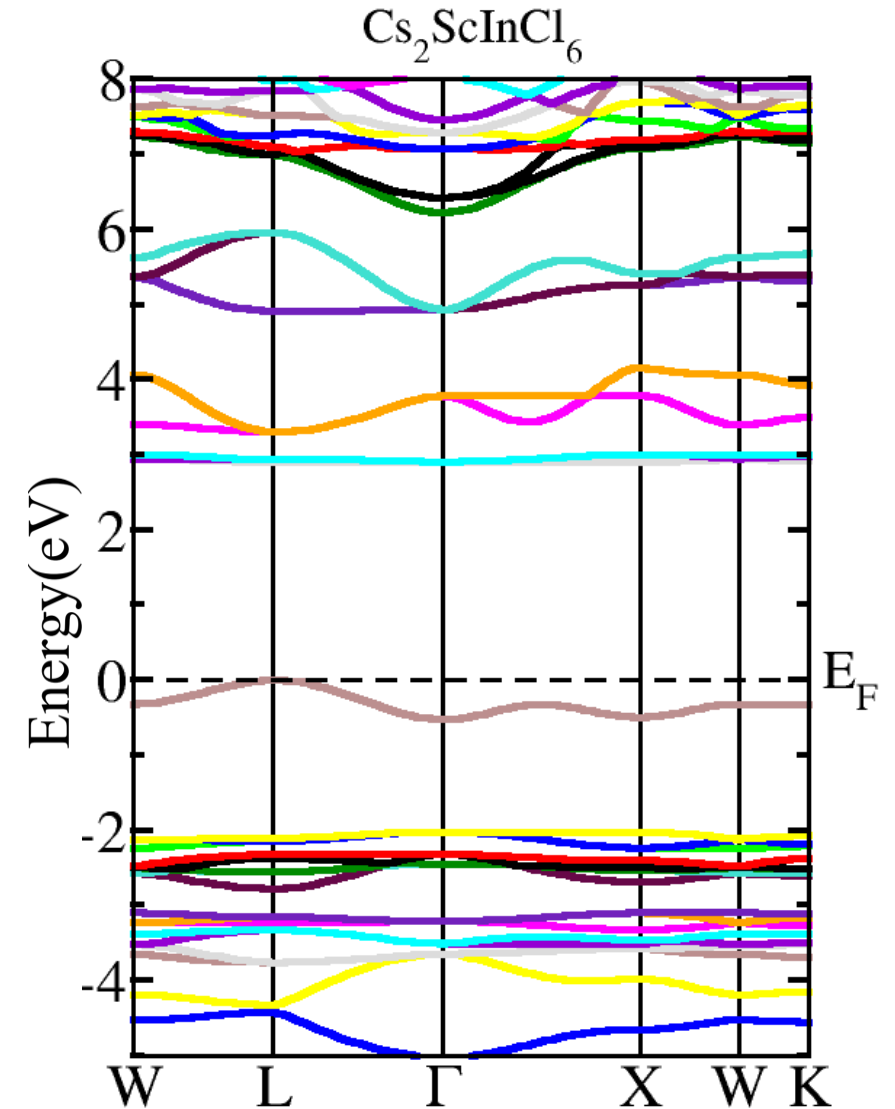
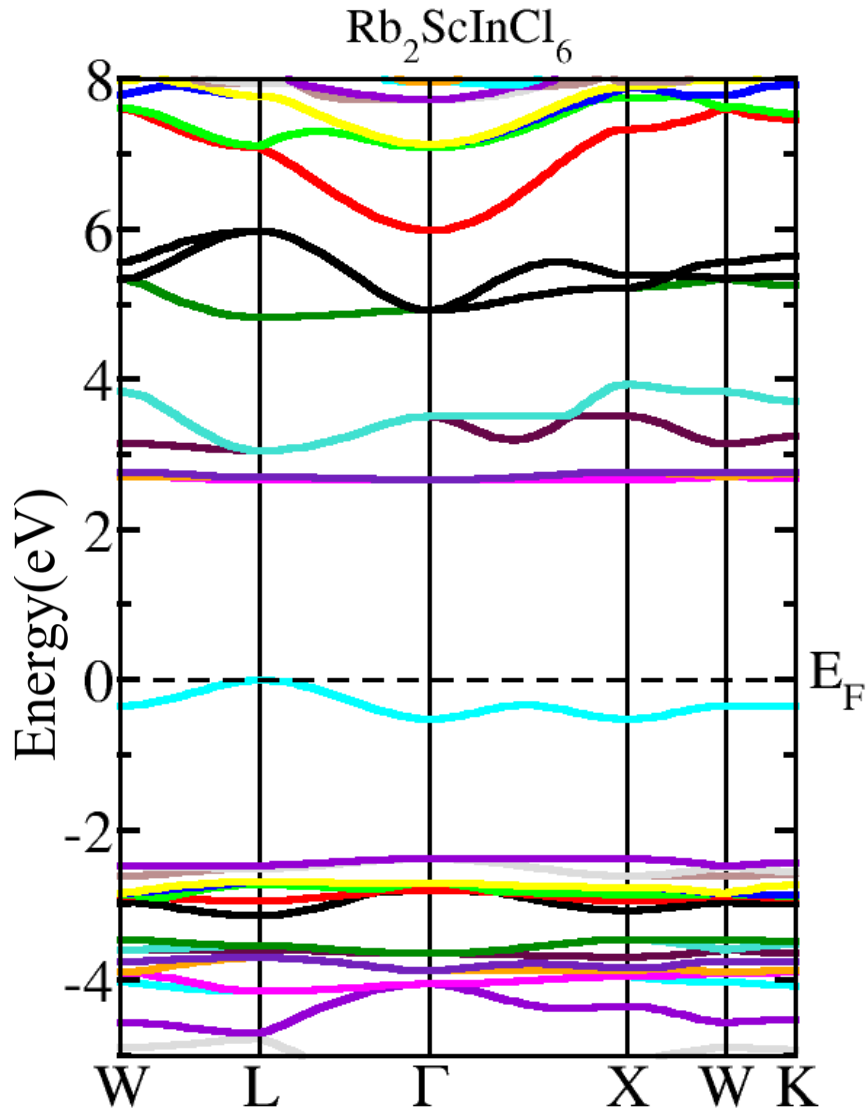
Optimized Lattice parameters



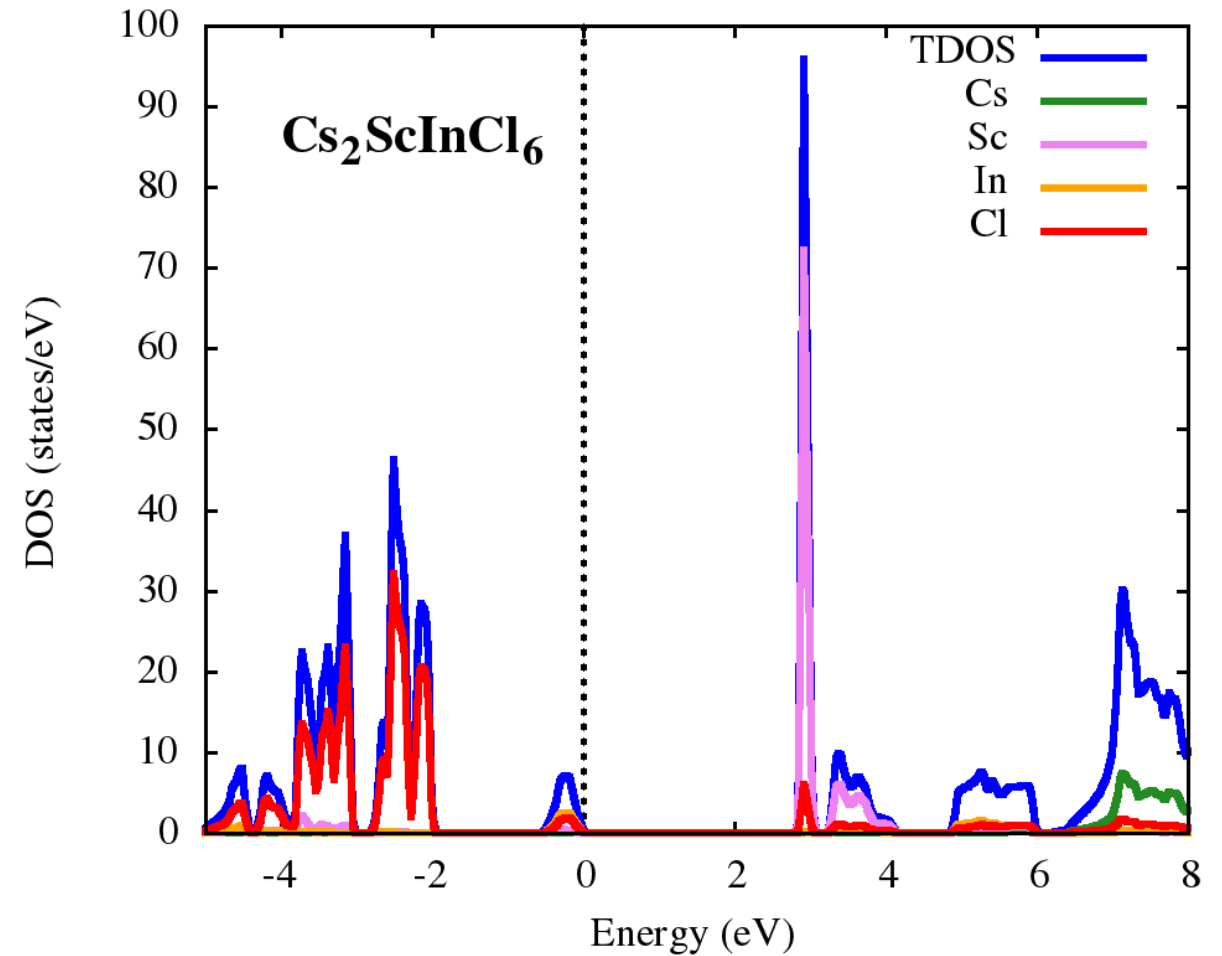
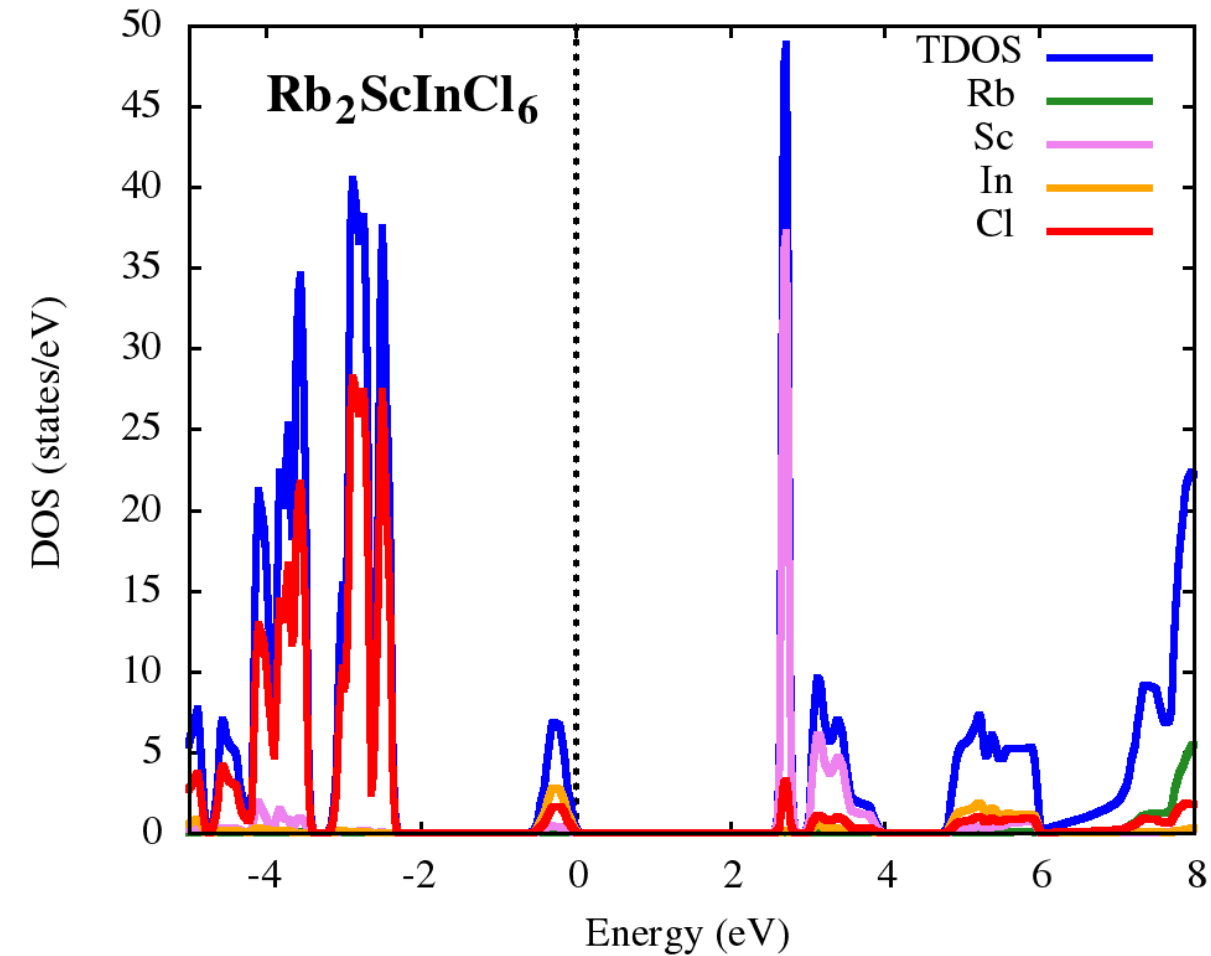
Optimized Lattice parameters

System	Lattice parameter (Å)	Band gap (eV)	
		PBE-GGA	TB-mBJ
$\text{Rb}_2\text{ScInCl}_6$	11.073	2.599	2.662
$\text{Cs}_2\text{ScInCl}_6$	11.163	2.802	2.902

Electronic properties

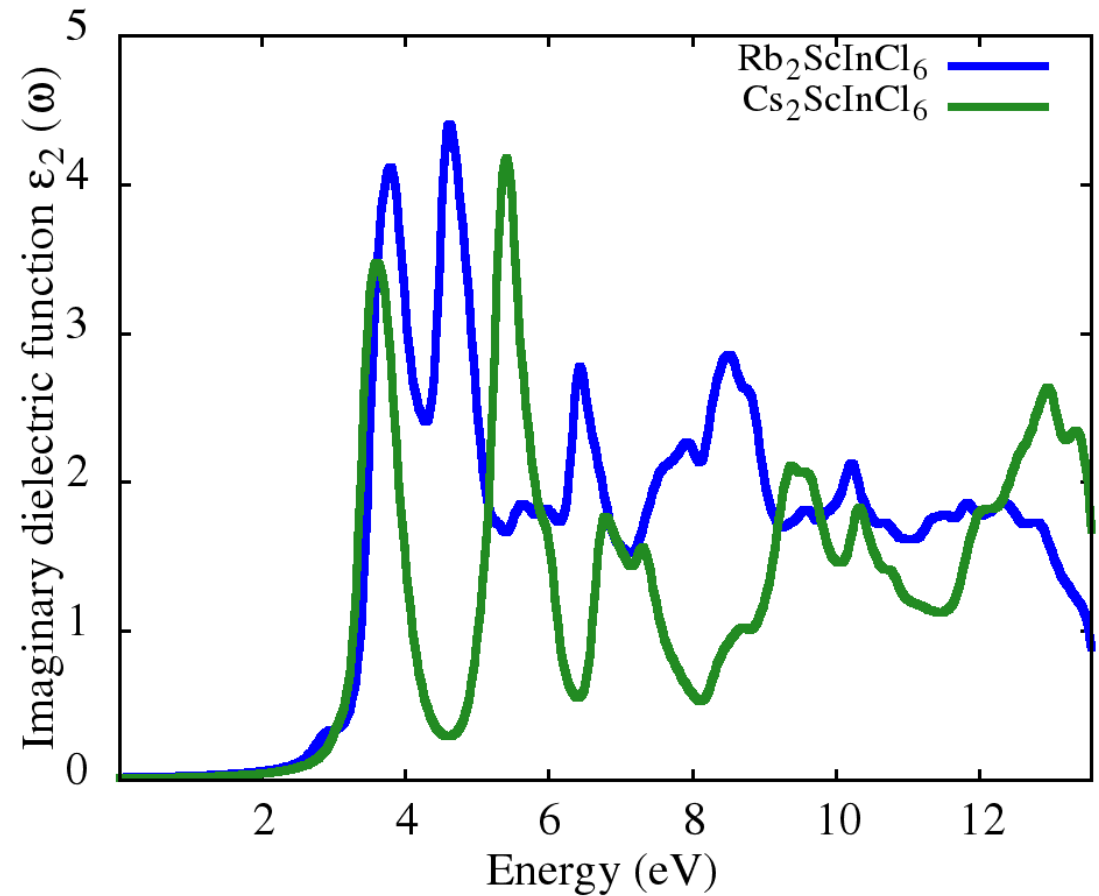
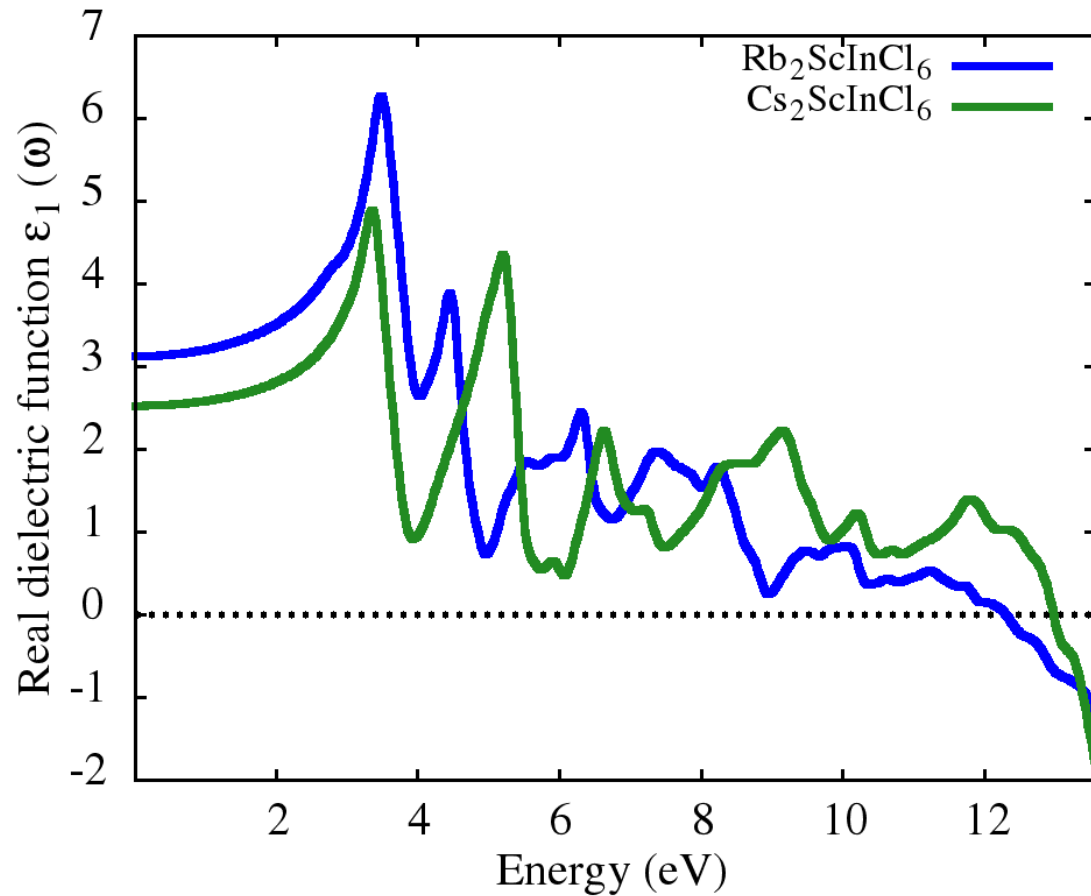


Electronic properties

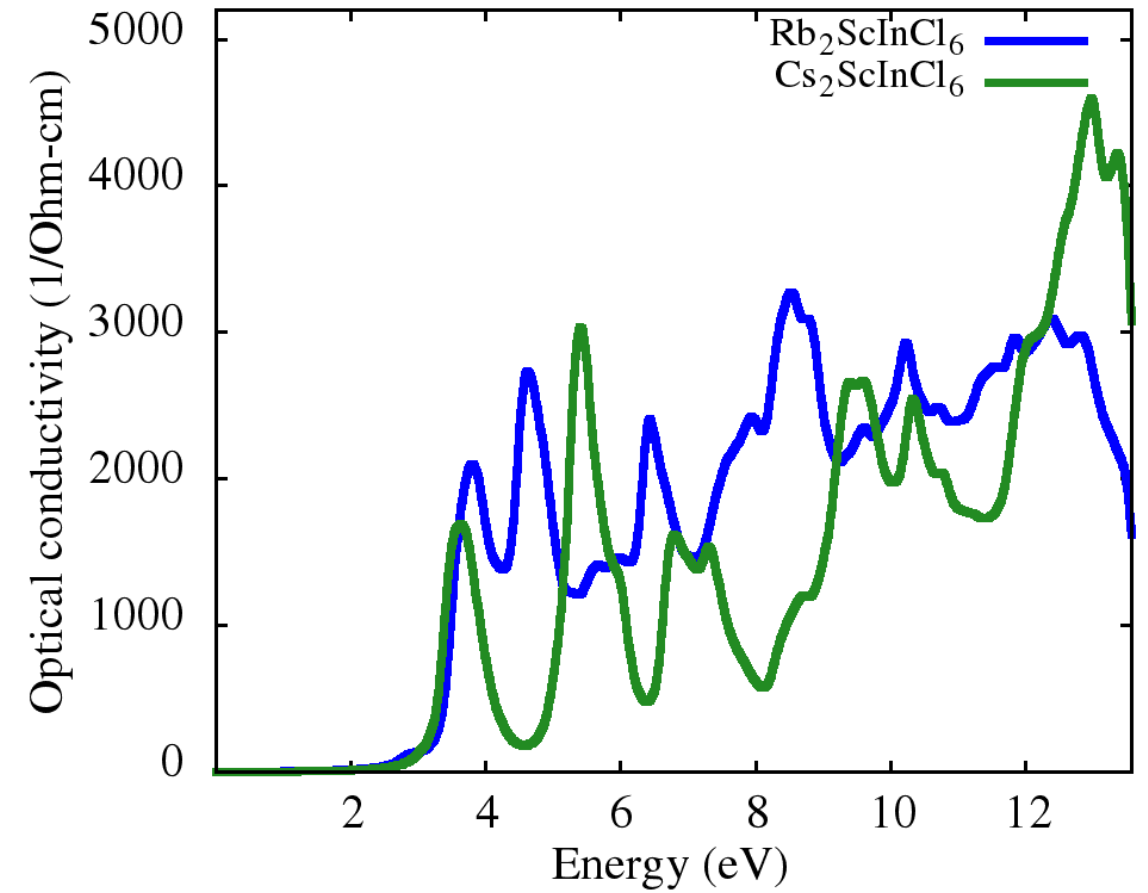
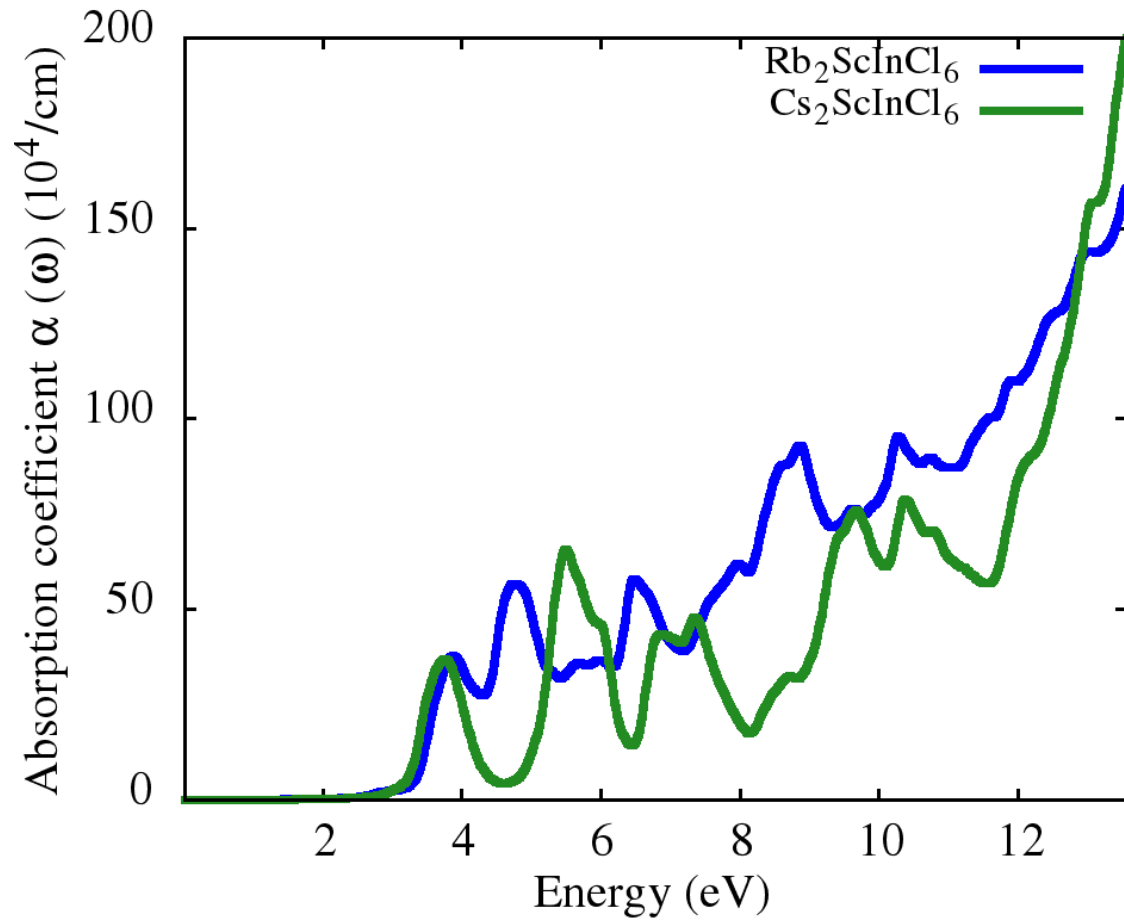


Optical properties

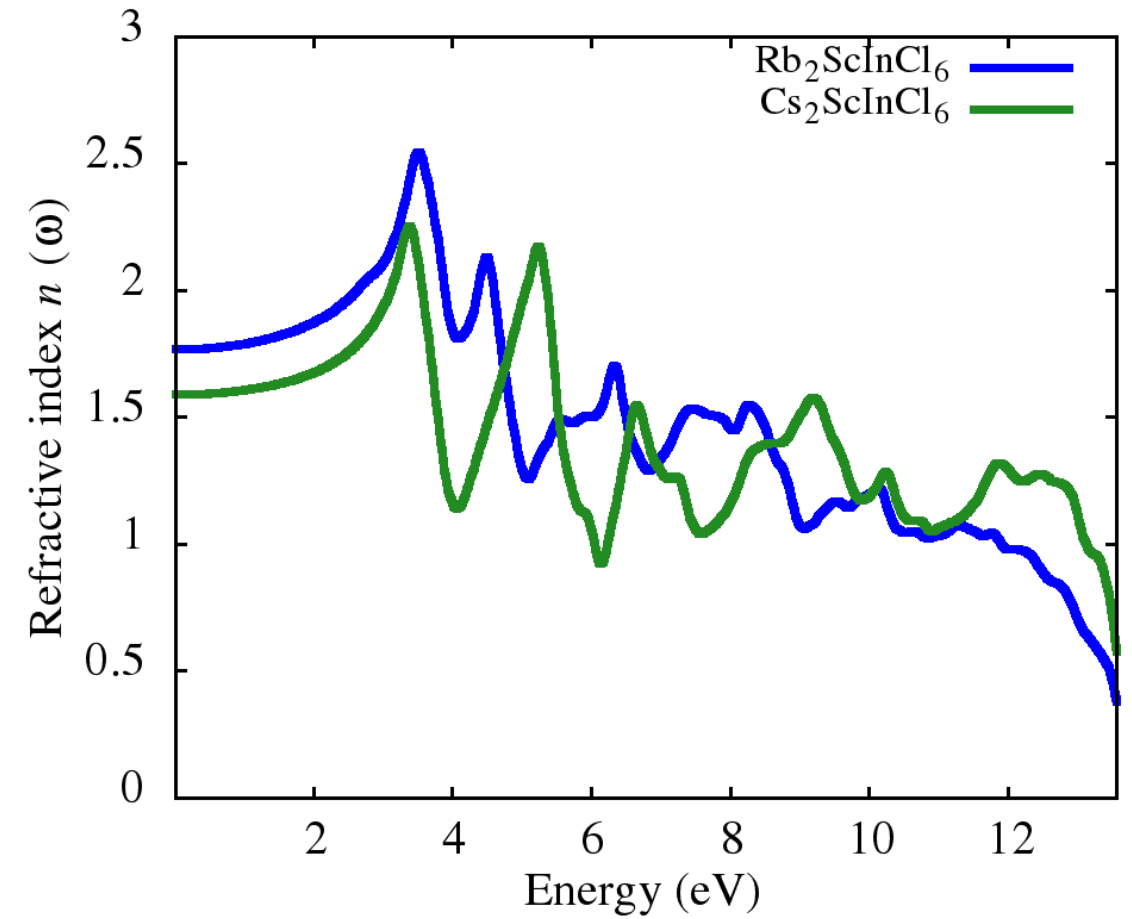
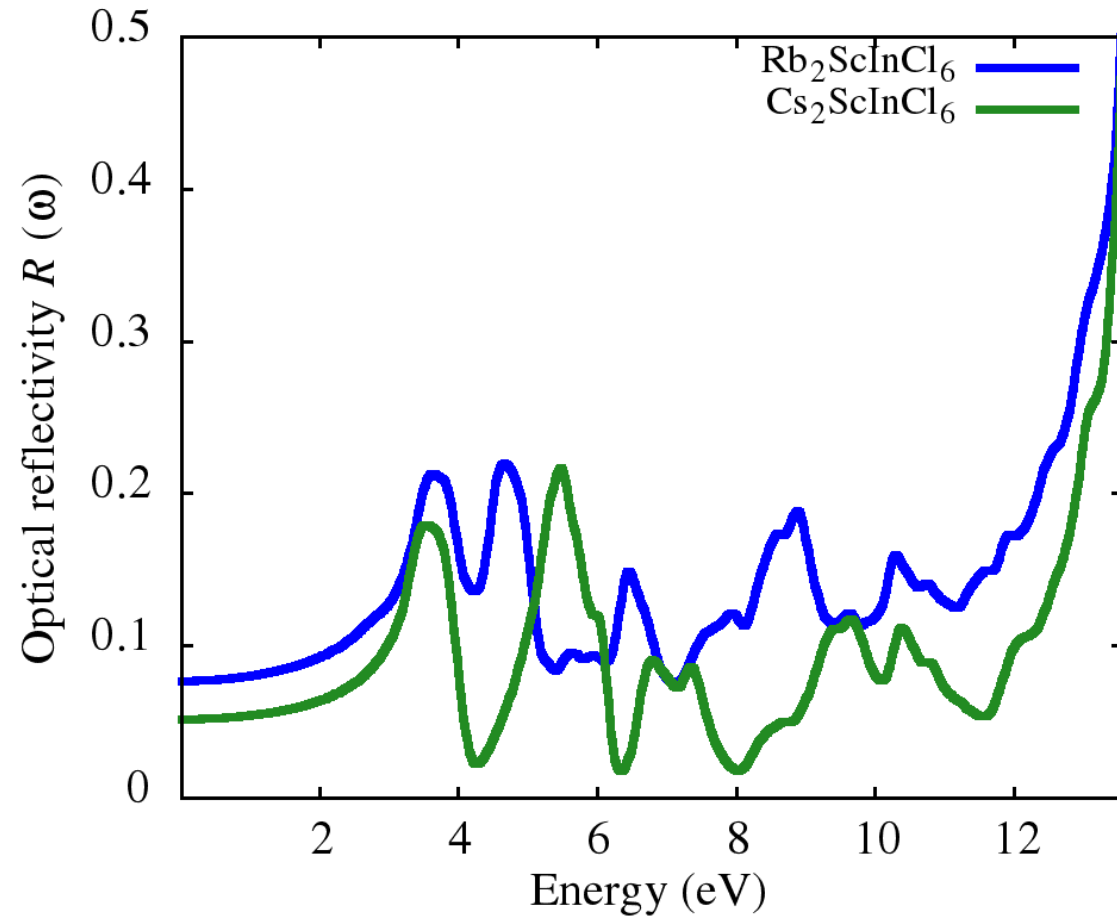
$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$



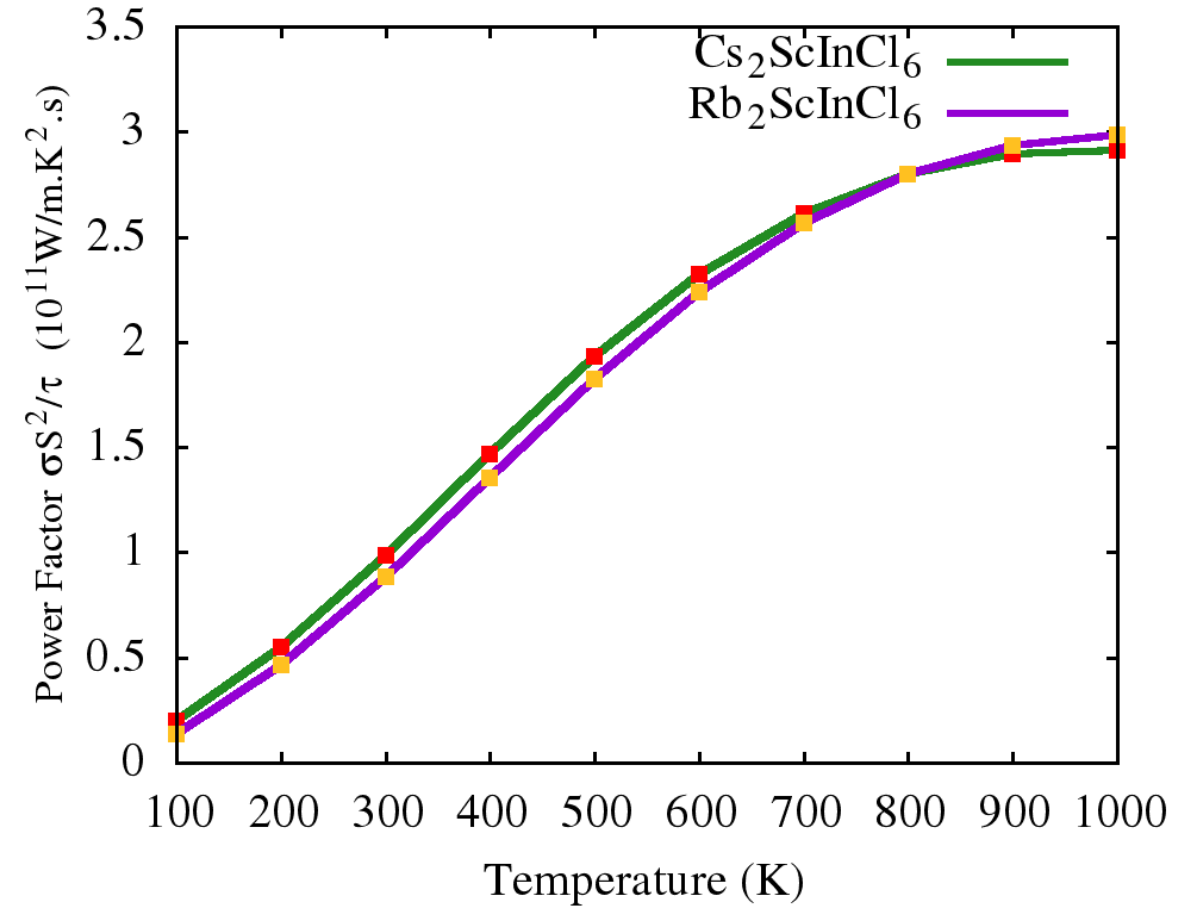
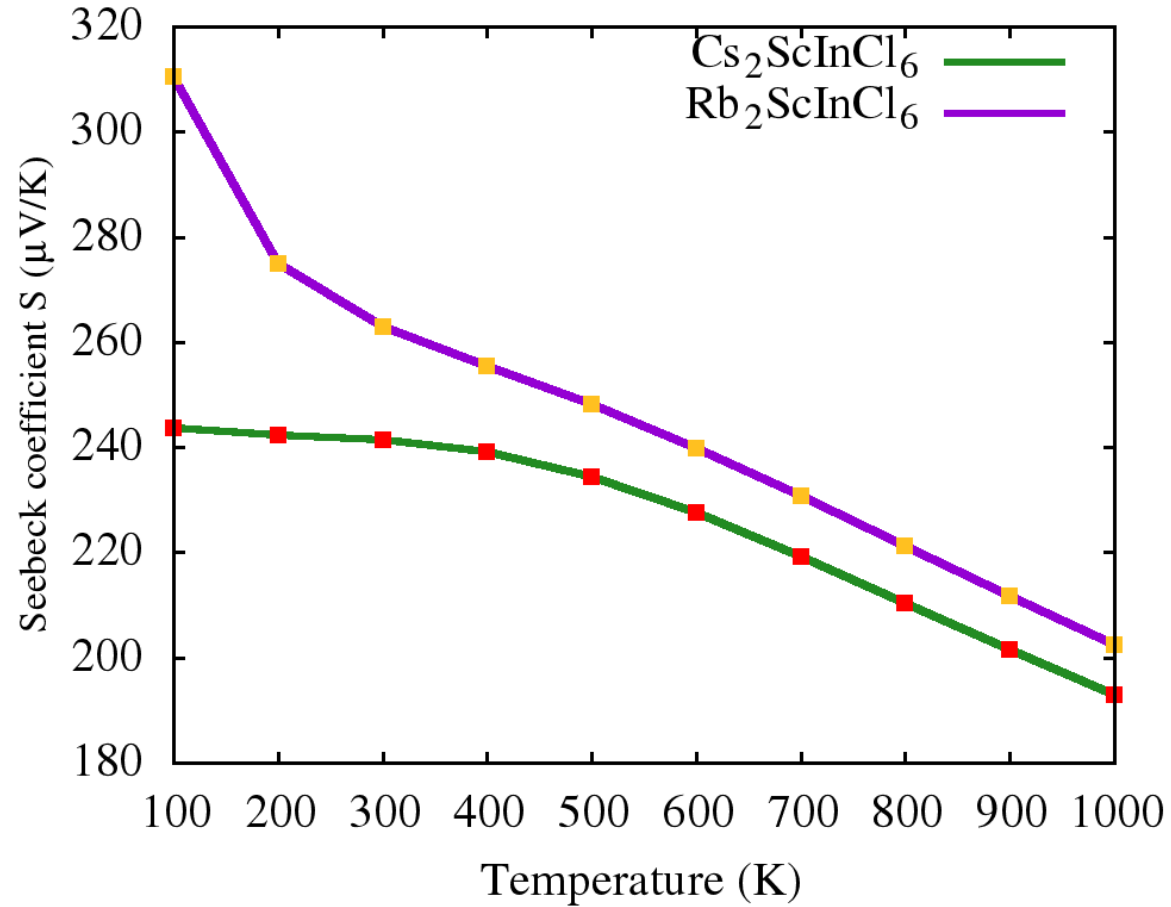
Optical properties



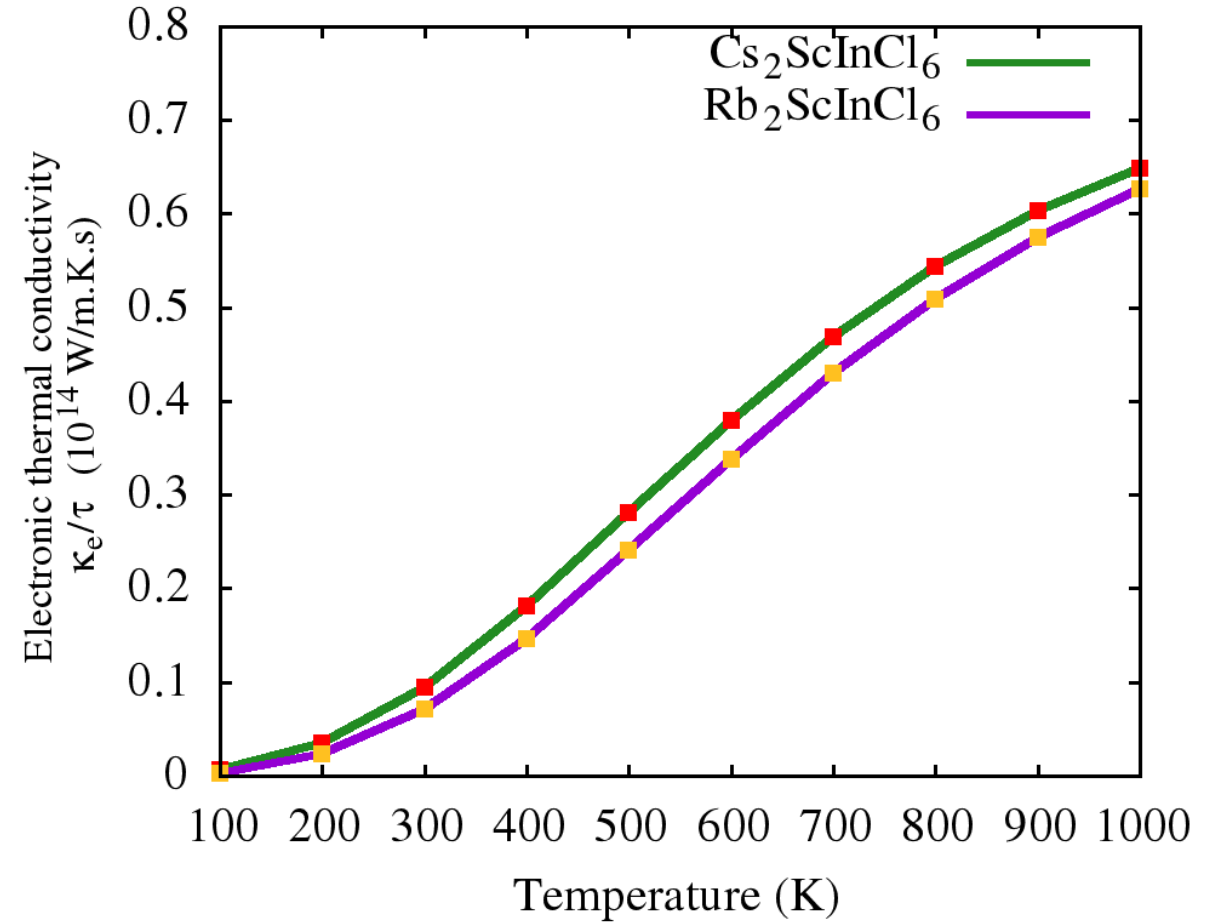
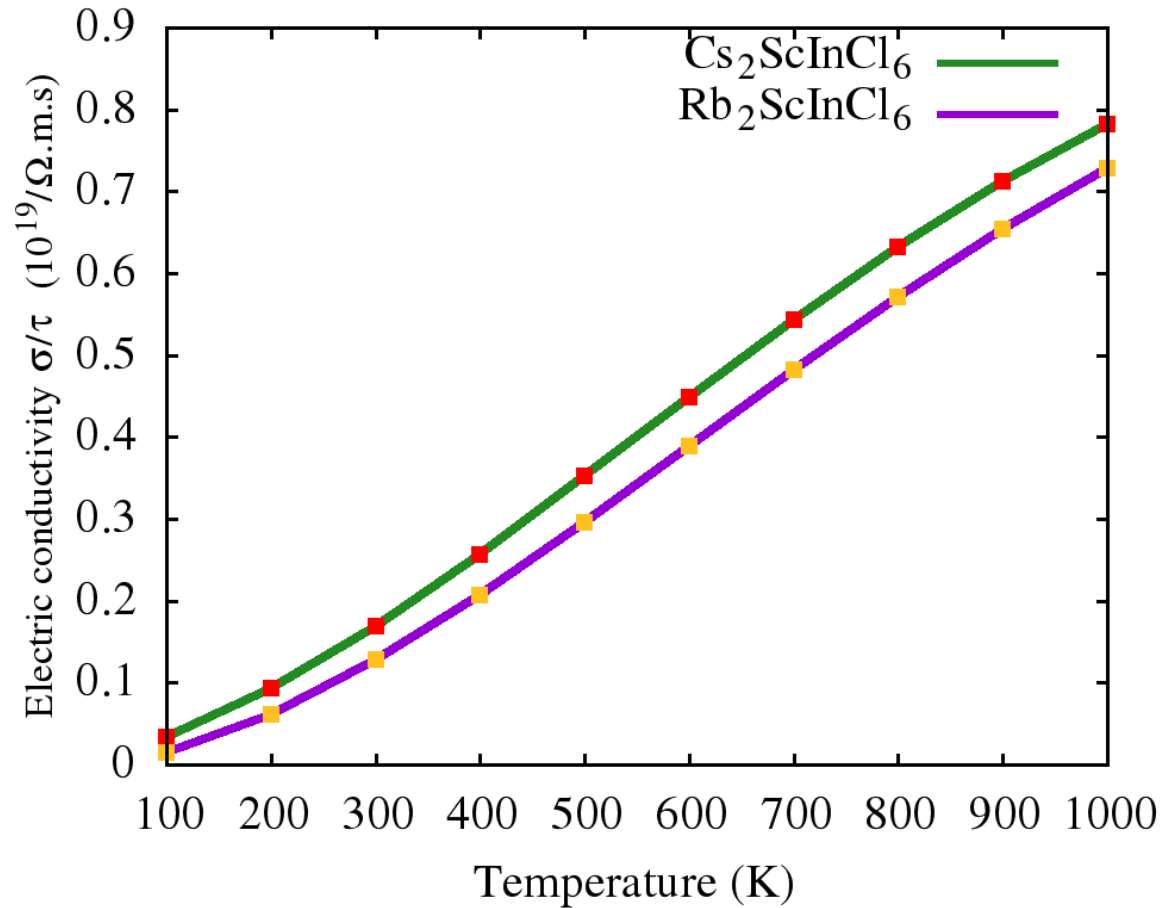
Optical properties



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”

