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Solid-solution modelling using first-principles methods: Case studies for $(Cu,Ag)_2ZnSnSe_4$ and $(FA,Cs)PbI_3$

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Our quest to find new materials to be utilised in technological applications leads us more and more towards solid solutions between different materials. These solid solutions allow for the fine-tuning of desired material properties, but also pose additional problems in experimental characterisation and theoretical modelling. While we're able to deal with fractional occupancies of Wyckoff positions in experimental investigations, this is not the case for theoretical materials modelling based on density functional theory, and we have to resort to additional methods to properly model the structural, electronic, and optical properties of solid solutions.

Here, we're using first-principles calculations based on density functional theory to shed some light into the structure-property relations in the $(Cu,Ag)_2ZnSnSe_4$ and $(FA,Cs)PbI_3$ solid solutions (FA: formamidinium). While $(Cu,Ag)_2ZnSnSe_4$ only requires the mixing over different Wyckoff positions, in $(FA,Cs)PbI_3$ we additionally have to account for the rotations of the FA cation. For both systems, in order to simulate the different concentrations within the solid solution, we're employing a supercell approach. All our structure models are geometry optimised employing the recently developed SCAN exchange and correlation functional. In order to obtain more reliable electronic and optical properties, selected optimised structures are subjected to one-shot calculations employing the more accurate hybrid functional HSE06.

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Primary author: Dr FRITSCH, Daniel (Helmholtz-Zentrum Berlin)

Co-author: Prof. SCHORR, Susan (Helmholtz-Zentrum Berlin)

Presenter: Dr FRITSCH, Daniel (Helmholtz-Zentrum Berlin)

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