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Ab-initio modeling of non-stoichiometric FeO_{1-x}S_x using the VCA approach

We present an ab-initio study of non-stoichiometric mixed iron oxide / sulfide using the virtual crystal approximation (VCA). This allows us to analyse the cell parameter, the bulk modulus and the density of states as a function of sulfur content.

Primary author: Mr MULAUDZI, Masilu Godfrey (Materials Modelling Center - University of Limpopo)

Co-author: Dr ACKERMANN, Lutz (Materials Modelling Center - University of Limpopo)

Presenter: Mr MULAUDZI, Masilu Godfrey (Materials Modelling Center - University of Limpopo)

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