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Fine-tuning the strategy XtalOpt + Gibbs2 codes. Application to thermoelectric compounds (AgCl, PbTe and CoSb3) under stress: Phase diagrams pT

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The ultimate objective of this work is the proposal of new materials with high thermoelectric performance. The success in its achievement is associated with the fulfilment of two other intermediate objectives. The first is of a methodological nature and consists on the combination of prediction models of crystalline structures with strategies for chemical-quantum calculation of electronic, thermodynamic and transport properties (VASP+newGIBBS). The second is of an applied nature. It seeks to obtain property-structure correlations from the computational exploration of regions of increasing pressures in the phase diagram of families of compounds with high value of the figure of merit (ZT) (AgCl, PbTe, SnSe, CoSb3) and allowing stoichiometric variations. The code XtalOpt is a computational tool that makes use of evolutionary algorithms for the prediction of crystal structures based solely on the composition of a material system. The number of atoms in the unit cell that handles. XtalOpt can reach a hundred. It has been created entirely of Prof. Eva Zurek. Its set up to couple it with the code GIBBS2 supposes a novel computational strategy in the search for stable structures in specific regions of the phase diagram, created in the group TCCMAT at the University of Oviedo. Hocine C has completed his PhD at the age of 45 years from Oviedo University, Spain. He is professor of Université des frere Mentouri, Constantine/Algeria. He has over 5 publications that have been cited over 20 times, and his publication H-index is 7.8.

Recent publications

1. Chorfi H, Lobato Á, Boudjada F, Salvadó MA, Franco R, Baonza VG, Recio JM. Computational Modeling of Tensile Stress Effects on the Structure and Stability of Prototypical Covalent and Layered Materials. Nanomaterials (Basel). 2019 Oct 18;9(10):1483. doi: 10.3390/nano9101483. PMID: 31635297; PMCID: PMC6835623.

2. Chorfi, H. (2020). Stress-strain relationships in 2D and 3D crystalline solids.

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