High Entropy Oxides; Microstructure, Ionic Conductivity and Simulation

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Abstract

The (Co,Cu,Mg,Ni,Zn)O HEOx and a series of samples doped with Li up to the upper limit of 30 at.%, $(Co,Cu,Mg,Ni,Zn)_{100-x}Li_xO$, were synthesized using the solid state synthesis. The mixtures of the starting components were calcined, in order to remove the CO_2 from the system, and then free sintered at 900 °C for 20 hours. The phase composition of the obtained materials was studied. The determined solubility limit of Li in the *Fm-3m* structure of (Co,Cu,Mg,Ni,Zn)O solid solution is much lower than it was already reported and noticeable content of Cu-Li spinel for the sample with 30 at.% of Li was observed. The ionic conductivities measured with the use of electrochemical impedance spectroscopy proved that the materials behave as an ionic conductor. The microstructure studies of obtained solid solutions suggest a new interpretation of the conductivity data and the use of advanced simulation techniques, namely the density functional theory, DFT.

DFT has been generalized to deal with many different situations including multicomponent systems. It is the most successful and also the most promising approach to compute the electronic structure of matter. In its original formulation, DFT provides the ground state properties of a system, and the electron density plays a key role in chemistry.

Here we will show the derivation schema, interpretation and perspectives of the recently formulated quaternion based DFT. Upon combining the final form of classical particle mechanics (the Hamilton–Jacobi Equation) and quaternion algebra we present the schema of rigorous derivation of the Schrödinger's mechanics [1]. We address some problems and paradoxes that emerge through conventional interpretations [2]. The fundamental consequences, the relation of the derived formulae to other instances of DFT and the future prospects are discussed.

Acknowledgements
This work is supported by a National Science Centre for OPUS 13, project no. 2017/25/B/ST8/02549.

References

[1] A. Karamatskou, H. Kleinert, Geometrization of the Schrödinger equation: Application of the Maupertuis Principle to quantum mechanics, Int. J. Geom Methods 11 (2014) 145006-1450017.

[2] M. Danielewski, L. Sapa, Nonlinear Klein-Gordon Equation in Cauchy-Navier Elastic Solid, Cherkasy Univ. Bulletin, Physical and Mathematical Sciences 1 (2017), 22–29.