excitation and has been widely used for televisions[2]. In this study we perform crystal structure prediction and investigate energy landscape of Yttrium Oxisulfide (Y_2O_2S). In order to predict new crystal structures, global optimizations on the energy landscape of Y_2O_2S has been performed. Afterwards, a local optimization has been performed using ab initio calculations. In particular various quantum mechanical methods have been applied: Density Functional Theory (DFT) with Local-Density Approximations (LDA) and Generalised Gradient Approximation (GGA), and hybrid B_3LYP (Becke, three-parameter, Lee-Yang-Parr) functional.

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Approximation and Error Prediction in Electrochemical Parameters Calculation Using Neural Networks

Vojislav V. Mitić[1,2],Branislav Ranđelović[1,3], Srdjan Ribar[4], Dušan Milošević[1],Branislav Vlahović[5], Hans Fecht[6], Markus Mohr[6]

[1]Faculty of Electronic Engineering, University of Nis, 14 Aleksandra Medvedeva, 18000 Nis, Serbia
[2]Institute of Technical Sciences of SASA, 35 Kneza Mihaila, 11000 Belgrade, Serbia
[3]Faculty of Teachers Education, University of K.Mitrovica, Nemanjina bb, 38218 Leposavic, Serbia
[4]Faculty of Mechanical Engineering, University of Belgrade, 16Kraljice Marije, 11000 Belgrade, Serbia
[5]North Carolina Central University, USA Durham NC, USA
[6]Institute of Multifunctional Properties of Materials, University of Ulm, Ulm, Germany

Various interesting results have been achieved in calculation of electrochemical parameters in nanomaterials, using neural networks. There appear some error, during those calculations, and it varies depending on number of neurons in layers. In this research we deal with errors, calculated for neural networks with *n=1,2…10*, neurons in first or second layer. We applied mean square approximation method, in order to get explicite formula for predicton of error, for other cases.