Structure prediction using global optimization and data mining in new Ce-O-N compounds

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Stable and metastable modifications inside of an ionic Ce-O-N compound with the compositions Ce_2ON_2 and Ce_3O_3N have been identified. The Ce_2ON_2 has been found as a best candidate with Ce^{4+} charge, even in the extreme conditions, [1,2] while Ce_3O_3N system is predicted for Ce^{3+} ions. Structure candidates for both compositions have been obtained after exploring the energy landscape for different pressure values and using empirical potentials. Global searches were performed on the enthalpy landscapes for three numbers of formula units per simulation cell (Z = 1, 2, 3), and for six different pressures (0, 0.016, 0.16, 1,6, 16, and 160 GPa) yielding a total of 14400 structure candidates for each composition. Additionally, potential structure candidates have been found using data mining of the ICSD database. We have extracted candidates that occur in the ICSD database with general formula A_2BC_2 and A_3B_3C, respectively. Energetically most favorable structure candidates obtained using the global search and the data mining were locally optimized on *ab initio* level in the sequence of the research. Local optimizations are performed. Finally, *ab initio* calculations of the total energy and local optimizations of the structure candidates were performed on the density functional theory level using the local density approximation (LDA) and the CRYSTAL17 code.

[1] J. Zagorac, J.C. Schön, B. Matović, T. Škundrić, D. Zagorac. Predicting Feasible Modifications of Ce_2ON_2 Using a Combination of Global Optimization and Data Mining. J. Phase Equilib. Diffus. 41, 538–549 (2020)

[2] J. Zagorac, D. Zagorac, D. Jovanović, M. Pejić, T. Škundrić, B. Matović, Ab Initio Investigations and Behaviour of the α-Ce2ON2 Phase in the Extreme Pressure Conditions. Journal of Innovative Materials in Extreme Conditions, 2, 36-43 (2021).