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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 Ce2ON2 and Ce3O3N have been identified. The Ce2ON2 has been found as a best candidate with Ce4+ charge, even in the extreme conditions, [1,2] while Ce3O3N system is predicted for Ce3+ ions. Structure candidates for both compositions have been obtained after exploring the energy landscape for different pressure values and using empirical potentials.

Primary author: Dr ZAGORAC, Jelena (INN Vinca, Belgrade, Serbia)

Co-authors: SCHOEN, Christian J. (Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany); Dr MATOVIC, Branko (INN Vinca, Belgrade, Serbia); Dr ZAGORAC, Dejan (INN Vinca, Belgrade, Serbia)

Presenter: Dr ZAGORAC, Jelena (INN Vinca, Belgrade, Serbia)

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