

Abstract Submitted
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Stability and Meta-stability of Clusters in a Reactive Atmosphere: Theoretical Evidence for Unexpected Stoichiometries of Mg_MO_x ¹
SASWATA BHATTACHARYA, SERGEY V. LEVCHENKO, LUCA M. GHIRINGHELLI, MATTHIAS SCHEFFLER, Fritz Haber Institute of the Max Planck Society — Applying genetic algorithm and replica exchange molecular dynamics in a cascade approach we calculate structure and composition of Mg_MO_x clusters at realistic temperatures and oxygen pressures. The cascade starts with force field and goes up to density functional theory with exact exchange plus correlation in the random phase approximation². The stable compositions are identified using *ab initio* atomistic thermodynamics. We find that at realistic environmental conditions small clusters ($M = 1-5$) are in thermodynamic equilibrium when $x > M$. Non-stoichiometric clusters are found to have in general higher spin multiplicity than stoichiometric ones. This suggests a possibility of tuning magnetic properties by changing environmental conditions.

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²X. Ren, P. Rinke, C. Joas, and M. Scheffler, Invited Review: Random-phase approximation and its applications in computational chemistry and materials science. *J. Mater. Sci.* **47**, 21 (2012).

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