UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

Seminar Theoretische Physik

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Computational Nano-Materials Design of Oxide-based Energy Saving Spintronics and Re-RAM Materials by Two-dimensional Spinodal Nano-decomposition:
Beyond-LDA and Multi-Scale Simulation

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Abstract:
Based upon self-interaction-corrected LDA and multi-scale simulation, I would like to discuss the computational nano-materials design of oxide-based energy saving spintronics materials by using the self-organized nano-structure of C, N, and cation vacancy-doped MgO, CaO, BaO, and ZnO without 3d transition atom doping. I will compare the theoretical predictions and design with the available experimental data. I also discuss the origin and switching mechanism of NiO-based Re-RAM materials caused by self-organized two-dimensional spinodal nano-decomposition.

Prof. Dr. P. Entel