Abstract Submitted
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Computational Nano-materials Design of Dynamically Created New Functional Ordered Oxide Nano-superstructures by Spinodal Nano-Decomposition: Design vs. Experimental Realizations MASAYOSHI SEIKE, TETSUYA FUKUSHIMA, KAZUNORI SATO, HIROSHI KATAYAMA-YOSHIDA, Osaka University — Based on ab initio electronic structure calculation and multi-scale simulation, we discuss the design of magnetic mechanism and the self-organized Spinodal Nano-Decomposition in dilute magnetic oxides in MgO, SrO, BaO, CaO, ZnO, NiO , and Re-RAM with d0 ferromagnetism. By controlling the dimensionality (2D and 3D) of the crystal growth, crystal growth speed, substrate temperatures, and seeding in the self-organized nanostructure formation, we design the shape controlled quantum-dot (Dairiseki-Phase) and quantum nanowire (Konbu-Phase), and the new functionality such a Re-RAM, and high-blocking temperature in super-para-magnetism. We compare our recent computational nano-materials design data with the recent available experimental verifications.

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Kazunori Sato
Osaka University

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