Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Computational Nano-materials Design for Spinodal Nanotechnology as a New Class of Bottom-up Nanotechnology HIROSHI KATAYAMA-YOSHIDA, TETSUYA FUKUSHIMA, Graduate School of Engineering Science, Osaka University, KAZUNORI SATO, Graduate School of Engineering, Osaka University — Based on the spinodal nano-decomposition (SND) of dilute magnetic semiconductors (DMS) [1,2], we generalized the SND to the application of catalysis [3,4] and photovoltaic solar-cells [5], where nano-scale particle formation in catalysis and and nano-scale separation of electrons and holes are essential in order to enhance the efficiency. First, we summarize the shape control (Konbu- & Dairiseki-Phases) and dimensionality dependence of crystal growth condition on SND in DMS. Second, we discuss the application of SND for the formation of nano-particles and the self-regeneration in three-way catalysis for automotive emission control by Perovskite La(Fe,Pd or Rh)O_3. Third, we propose (i) self-regeneration mechanism and (ii) self-organized nano-structures by SND in chalcopyrite Cu(In,Ga)Se_2, Kesterite $Cu_2ZnSnSe_4$, and Perovskite $CsSnI_3$ for the low-cost, environment-friendly and high-efficiency photovoltaic solar cells using first-principles calculations. [1] K. Sato et al., Rev. Mod. Phys., 82, 1633 (2010). [2] T. Dietl, et al., Rev. Mod. Phys., (2015) in press. [3] H. Kizaki et al., Chem. Phys. Lett. 579, 85 (2013). [4] I. Hamada et al., J. Am. Chem. Soc. 133, 18506 (2011). [5] Y. Tani et al., Appl. Phys. Express, 3, 101201 (2010).

Hiroshi Katayama-Yoshida
Graduate School of Engineering Science, Osaka University

Date submitted: 07 Nov 2015 Electronic form version 1.4