

Rampi Ramprasad Publications

2010

Submitted Publications:

H. Zhu, C. Tang and R. Ramprasad, "**Phase equilibria at Si-HfO₂ and Pt-HfO₂ interfaces from first principles thermodynamics**".

G. Pilania and R. Ramprasad, "**Complex Polarization Ordering in PbTiO₃ Nanowires: A First Principles Computational Study**".

G. Pilania and R. Ramprasad, "**Adsorption of atomic oxygen on cubic PbTiO₃ and LaMnO₃ (001) surfaces: A density functional theory study**".

Publications:

T. Sadowski and R. Ramprasad, "**First Principles Computational Study of Wurtzite CdTe Nanowires**", *J. Mater. Sci.*, 45, 5463 (2010).

L. Dong, S. K. Yadav, R. Ramprasad, and S. P. Alpay, "**Band gap tuning in GaN through equibiaxial in-plane strains**", *Appl. Phys. Lett.*, 96, 202106 (2010).

S. K. Yadav, T. Sadowski and R. Ramprasad, "**Density functional theory study of ZnX (X=O, S, Se, Te) under uniaxial strain**", *Phys. Rev. B*, 81, 144120 (2010).

C. Tang, and R. Ramprasad, "**Point defect chemistry in amorphous HfO₂: Density functional theory calculations**", *Phys. Rev. B*, 81, 161201(R) (2010).

T. Sadowski, and R. Ramprasad, "**Ab Initio Thermodynamic Model to Assess Stability of Heterostructure Nanocrystals**", *Appl. Phys. Lett.*, 96, 101906 (2010).

J. D. Doll, G. Pilania, R. Ramprasad and F. Papadimitrakopoulos, "**Oxygen-Assisted Unidirectional Growth of CdSe Nanorods Using a Low-Temperature Redox Process**", *Nano Lett.*, 10 (2), 680 (2010).

T. Sadowski, and R. Ramprasad, "**Core/Shell CdSe/CdTe Heterostructure Nanowires Under Axial Strain**", *J. Phys. Chem. C*, 114, 1173 (2010).

M. E. Stournara and R. Ramprasad, "**A first principles investigation of isotactic polypropylene**", *J. Mater. Sci.* 45, 443 (2010).

BOOK CHAPTER: R. Ramprasad, N. Shi and C. Tang, "**Modeling the physics and chemistry of interfaces in nanodielectrics**", in *Dielectric Polymer Nanocomposites* (Ed. J. K. Nelson), Springer (2010).

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H. Zhu, M. Aindow and R. Ramprasad, "**Stability and work function of TiCxN1-x alloy surfaces: Density functional theory calculations**", *Phys. Rev. B* 80, 201406

G. Pilania, S. P. Alpay and R. Ramprasad, "**Ab initio study of ferroelectricity in BaTiO3 nanowires**", *Phys. Rev. B* 80, 014113 (2009).

G. Pilania, D. Q. Tan, Y. Cao, V. S. Venkataramani, Q. Chen and R. Ramprasad, "**Ab initio study of antiferroelectric PbZrO3 (001) surfaces**", *J. Mater. Sci.* 44, 524

G. Pilania, T. Sadowski and R. Ramprasad, "**Oxygen adsorption on CdSe Surfaces: A case study of asymmetric anisotropic growth through Ab initio computations**", *J. Phys. Chem. C.* 113(5), 1863 (2009).

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R. Ramprasad and C. Tang, "**Circuit elements at optical frequencies from first principles: A synthesis of electronic structure and circuit theories**", *J. Appl. Phys.*, **100**, 034305 (2006).

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Patents

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