

A. PEER REVIEWED JOURNAL ARTICLES (# indicates corresponding author):

Submitted

95. R.J. Bondi, S. Lee, and **G.S. Hwang**[#], "First-principles study of the mechanical and optical properties of amorphous hydrogenated silicon and silicon-rich silicon oxide," submitted (2009).
94. S.H. Lee, J.A. Stephens, and **G.S. Hwang**[#], "On the Nature and Origin of Si Surface Segregation in an Amorphous Au-Si alloy," submitted (2009).
93. N. Kong[#], T.A. Kirichenko, **G.S. Hwang**, and S.K. Banerjee, "Arsenic-Defect Complexes at SiO₂/Si Interfaces," *Phys. Rev. B*, under revision (2009).
92. S. Lee, R.J. Bondi, and **G.S. Hwang**[#], "Nature and Formation of Vacancy Defects in Silicon," *Phys. Rev. B*, under revision (2009).

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85. R.J. Bondi, S. Lee and **G.S. Hwang**[#], "Prediction of the Formation of Stable Periodic Self-Interstitial Chains [(I₄)_m, m=1-4] in Si under Biaxial Strain," *Appl. Phys. Lett.* **94**, 264101 (2009).
84. C.-L. Kuo and **G.S. Hwang**[#], "Structure and Diffusion of Boron in Amorphous Silica: Role of Oxygen Vacancy Related Defects," *Phys. Rev. B* **79**, 165201 (2009).
83. R. J. Bondi, S. Lee, and **G.S. Hwang**[#], "Biaxial Strain Effects on the Structure and Stability of Self-Interstitial Clusters in Silicon," *Phys. Rev. B* **79**, 104106 (2009).

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B. PATENTS/DISCLOSURES:

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2. "Method for Predicting the Behavior of Dopant and Defect Components," US Patent No. **US 7074270 B2**, 2006, with S. Yuzuru, U. Masamitsu, and W. A. Goddard III.
3. "Method for Predicting the Synthesis, Structure and Properties of Si Nanocrystals Embedded in Oxide Matrices," US Patent, *pending*, with D. Yu.
4. "First-principles Model for Predicting the Evolution of N-type Dopant Concentration and Electrical Activity Profiles in Ultrashallow Junction Formation," US Patent, *pending*, with S. Harrison.

C. BOOK CHAPTERS AND REVIEWS:

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2. **G.S. Hwang**, "Minireviews: Dynamics and Reactivity of Molecular Oxygen on Oxide Materials," ChemPhysChem, in preparation; invited.