

Mina Yoon
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(a) Professional Preparation

Ewha Womans University	Seoul, South Korea	Physics	B.S. in 1996
Seoul National University	Seoul, South Korea	Physics	M.S. in 1999
Michigan State University	East Lansing, MI, U.S.A.	Physics	Ph. D in 2004

(b) Appointments

- Joint Faculty, Professor, Department of Physics and Astronomy, University of Tennessee (UTK), Knoxville, TN, U.S.A., since December 2015
- R & D Scientist, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, U.S.A., since June 2009
- Research Assistant Professor, UTK, Nov. 2005 to June 2009
- Postdoc, ORNL, Sep. 2004 – Oct. 2005

(c) Selected Publications (Total 90 publications, over 4683 citations, h-index 35)

- “GPGPU Acceleration of All-Electron Electronic Structure Theory Using Localized Numeric Atom-Centered Basis Functions”, W.P. Huhn, B. Lange, V. W-z Yu, M. Yoon, V. Blum (submitted *Comp. Mat. Sci.* 2020) <https://arxiv.org/abs/1912.06636>.
- “Metastable $\text{Li}_{1-x}\text{Mn}_2\text{O}_4$, ($0 \leq x \leq 1$) spinel phases revealed by in-situ neutron diffraction and first-principles calculations”, B. Song, G. M. Veith, J. Park, M. Yoon, P. Whitfield, M. Kirkham, J. Liu, R. Schmidt, A. Huq, *Chem. Mat.* **31**, 124 (2019).
- “First-Principles Prediction of New Electrides with Nontrivial Band Topology Based on One-Dimensional Building Blocks”, C. Park, S.W. Kim, M. Yoon, *Phys. Rev. Lett.* **120**, 26401 (2018).
- “Predictive power of density functional theory in finite-temperature hydrogen adsorption/desorption thermodynamics with corrective energies and potential surfaces”, Y. Ihm, C. Park, J. Morris, J. H. Shim, Y.-H. Kim, B. G. Sumpter, and M. Yoon, *J. Phys. Chem. C* **122**, 26189 (2018).
- “First-principles Prediction of Thermodynamically Stable Two-Dimensional Electrides”, W. Ming, M. Yoon, M.-H. Du, K. Lee, and S. W. Kim, *J. Am. Chem. Soc.* **138**, 15336 (2016).
- “Alloy Engineering of Defect Properties in Semiconductors: Suppression of Deep Levels in 2D Transition-metal Dichalcogenides”, B. Huang, M. Yoon, B. G Sumpter, S.-H. Wei, and F. Liu, *Phys. Rev. Lett.* **115**, 126806 (2015).
- “Growth of Metal Phthalocyanine on Deactivated Semiconducting Surfaces Steered by Selective Orbital Coupling”, S. R. Wagner, B. Huang, C. Park, J. Feng, M. Yoon, P. Zhang, *Phys. Rev. Lett.* **115**, 096101 (2015).
- “Electronic properties of bilayer graphenes strongly coupled to interlayer stacking and an external electric field”, C. Park, J. Ryou, S. Hong, B. Sumpter, G. Kim, M. Yoon, *Phys. Rev. Lett.* **115**, 015502 (2015).

(d) Synergistic Activities

- Max Planck Fellowship, Theory Department, Fritz Haber Institute of the Max Planck Society, Berlin, Germany, Aug. 2008 to June 2011
- Editorial Board - Dataset Papers in Nanotechnology (since 2012); Journal of Theoretical Chemistry (2012-2017); The Scientific Pages of Atoms and Molecules (since 2017); The journal of Chemistry: Theoretical Chemistry (since 2017); Annals of Atoms and Molecules (since 2017).
- Referee for journals: Nature, Science, Physical Review Letters, Journal of the American Chemical Society, Physical Review B, Nano Letters, Journal of Chemical Physics, Nanotechnology, ACS

Nano, Applied Physics Letters, Physics Letters A, Journal of Physics: Condensed Matter, Chemistry of Materials, Chemical Physics Letters, etc.

- Reviewer of DOE grant proposals and LDRD Seed proposals at ORNL
- Organizing conferences – Organizer of a symposium on “Agile Design of Electronic Materials: Aligned Computational and Experimental Approaches” at the Electronic Materials Applications conference, sponsored by the American Ceramics Society, Orlando, Florida, January 2018, 2019, 2020; Organization committee of Advance Materials Congress 2017-2018; Co-organizer of a symposium on “Recent Advances in Computer-aided Materials Design” at Materials Science & Technology 2017, Oct. 8-12, 2017, Pittsburgh PA; Organizer of a symposium on “Computational Design of Electronic Materials” at the Electronic Materials and Applications Conference (EMA), sponsored by the American Ceramic Society, Orlando, Florida, January 2018; January 2017; Organizer 2016; Organizer 2015; co-Organizer, Jan 2014; Organization Committee, Conference on Computational Physics 2011, Gatlinburg, Tennessee (2011); Organizer, CECAM Workshop on First Principles Theory and Modeling in Organic Electronics, Lausanne, Switzerland (2011); Organizer, CECAM Symposium at Psi-k 2010 on Organic Electronics for Energy Research, Berlin, Germany (2010)
- Thesis advisor and postgraduate-scholar sponsor:
8 students; 7 postdoctoral scholars