Winter 2026 Colloquium
Materials Department

Professor Andrew M. Rappe

University of Pennsylvania

Friday, January 23, 2026

11:00 am | ESB 1001

Theoretical and Computational Materials Design of Functional and Smart Materials

In many fields of materials science, new materials are urgently needed. Advances in computers, algorithms, and changes in how we interact with data have brought about an inflection point in materials discovery. In this talk I will describe how theoretical physical insight and computational materials design now form an innovation loop that is tightly coupled with experimental advances. In this talk I will take the design of next-generation ferroelectrics as a key study target.

Within the past few years, we are experiencing a resurgence of interest in ferroelectrics due to the discovery of ferroelectricity in new material classes, including fluorites and wurtzites, which host novel complex mechanisms of ferroelectricity. Because fluorite HfO2 and wurtzite AlN are compatible with back end of the line growth onto prepared silicon computer chips, these materials are of great interest. Atomistic simulations of the mechanisms of ferroelectricity in these materials are crucial for future material and device engineering to both improve the material composition and design devices around the unique material properties.

In next generation ferroelectrics, the switching is essentially completely different than in perovskites. We study how the multiple order parameter nature of HfO2 and (Hf_{1-x}Zr_x)O_2 leads to a complex variety of different domain wall types, which we portray via a "lego block" formalism. Understanding this variety and the domain wall reactions that result leads to a new understanding of wake up and fatigue in HfO2 ferroelectrics.

To model ferroelectric switching in wurtzite AlN with the accuracy of DFT on a large scale, we trained a machine learned classical force field (MLFF) built on artificial neural networks. By training off the atomic positions and energies of thousands of DFT snapshots, our MLFF can be locally as accurate as DFT while allowing us to study large-scale switching phenomena.

We find emergent snowflake-like fractal regions that go from the atomic scale to nm scale. In our Monte Carlo modeling of these events, we see that these switching rules break the assumptions in the well-known KAI model for domain growth, with the fractal combinations causing faster switching toward the end.

Bio

Andrew M. Rappe is Blanchard Professor of Chemistry and Professor of Materials Science and Engineering at the University of Pennsylvania. He received his A.B. in “Chemistry and Physics” summa cum laude from Harvard University in 1986 and his Ph.D. in “Physics and Chemistry” from MIT in 1992, and was an IBM Postdoctoral Fellow at UC Berkeley before starting at Penn in 1994. Andrew received an NSF CAREER award in 1997, an Alfred P. Sloan Research Fellowship in 1998, and a Camille Dreyfus Teacher-Scholar Award in 1999, and was named a Fellow of the American Physical Society in 2006. Rappe was named Weston Visiting Professor at the Weizmann Institute of Science in 2014 and was awarded the Humboldt Research Award in 2017. Andrew is one of two founding co-directors of the VIPER honors program at Penn, the Vagelos Integrated Program in Energy Research, and has published more than 300 peer-reviewed articles, becoming a leader in the theory of hybrid organic-inorganic perovskites and of topological materials and championing the use of the bulk photovoltaic effect for solar energy harvesting.
https://www.chem.upenn.edu/profile/andrew-m-rappe

Hosted by Vojtech Vlcek.