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First-principles prediction of molecular piezoelectrics for nanoelectromechanical systems

Developing an atomistic understanding of electromechanical responses is a prerequisite for the bottom-up design of nanoelectromechanical systems. This presentation focuses on atomistic simulations of piezoelectric responses in aperiodic systems such as molecules, nanoparticles, or biomolecule agglomerates. More specifically, we develop an analytical approach to predict molecular piezoelectric coefficients from first principles (density functional theory) and introduce a formalism that unifies the description of molecular and mesoscopic responses. Based on this new approach, we develop computational procedures that expedite the first principles calculation of piezoelectric tensors for molecular systems. Numerical benchmarks demonstrate that the results from our analytical theory are fully consistent with numerical computations at drastically reduced computational cost. Most importantly, our approaches (i) reduce the time for developing new candidates from months in the laboratory down to hours and (ii) have the potential to be truly predictive even in the absence of experimental data.

Speaker Biography

Daniel S Lambrecht has completed his Ph.D from the University of Tuebingen, Germany, and performed his postdoctoral research at the University of California, Berkeley, USA. He is an Assistant Professor of Chemistry at the University of Pittsburgh, USA. He has over 35 publications that have been cited over 2,100 times, and his publication H- and i10-index are 19 and 26, respectively. He has received several national recognitions, including a 2017 Cottrell Scholar Award from the Research Corporation for Science Advancement, USA, and a Kekulé Award from the Association of Chemical Industry (VCI), Germany.

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