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Theory and modeling of piezoelectricty for nanomaterials

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Experiments have shown a great potential on electricity generation, especially piezoelectricity at nanoscale. Developing novel technologies for nano-devices is crucial for applications in biomedical sensing, environmental monitoring and personal electronics. Miniaturization of self-powering devices is the key challenge both experimentally and theoretically. Various approaches have been developed for harvesting energy from the environment based on thermoelectricity and piezoelectricity. Limited by the massive number of degrees of freedom at atomistic scale, an efficient and reliable theory and computational scheme are still out of reach. We developed Coarse-Grained Nonequilibrium Molecular Dynamics (CG-NEMD) under the framework of Finite Element Method and shape function, cluster calculation on interatomic force interaction to avoid ghost force, modified Nosè-Hoover Thermostate for temperature control and further extended the algorithm to nano-electrodynamics based on lattice dynamics and statistical mechanics. Through the theoretical formulation, atomistic representations of fundamental physical quantities, including polarization, electric potential and electric field, are defined. Balance laws for Nanoelectrodynamics are also formulated. Examples are presented to show the polarization and induced potential distribution in a Barium Titanate ($BaTiO_3$) nanocube. The simulation result shows that a great energy source hidden at nanoscale. A 6 nm cube can potential generate around 27 volts. The threshold of nano-piezoelectricity is also discovered. The possible applications of nanopiezoelectricity are also discussed.

Biography

James M. Chen is an Assistant Professor of Mechanical Engineering and Material Science at Pennsylvania State University, the Altoona College. He received his BS from National Chung-Hsing University in Taiwan in 2005, MS from National Taiwan University in Taiwan in 2007 and Ph.D. from The George Washington University in 2011. From 2007 to 2008 before starting his Ph.D. study, he was a research assistant in Institute of Physics, Sinica Academia in Taiwan conducting theoretical and experimental research in biophysics and electrodeless dielectrophoresis. Upon receiving his Ph.D. degree, he was a Visiting Assistant Professor at Indiana University-Purdue University Fort Wayne (IPFW). His research interest spans from biophysics, multiscale modeling of materials and mechanics, material science, nanoelectrodynamics, computational fluid dynamics and renewable energy. He is chosen as an Honorary Fellow at Australian Institute of High Energetic Materials (AIHEM) in 2011, has published more than 15 peer reviewed articles and has served in the editorial board of two leading journals, Nanoscience and Nanotechnology and Journal of Advanced Mathematics and Applications.

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