Multiscale Modeling of Nano-Biosensors

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Ultrasensitive nano-biosensor related research is a vital and rapidly developing field owing to its potential social and economic impact. Chemo-bio-mechanical phenomena in biosensing offer an enticing opportunity for researchers in the field of computational mechanics to investigate these phenomena with methodologies that have not previously been exploited and to furthermore provide new insight for designing next-generation ultrasensitive nano-biosensors. In this talk, I will highlight some recent advance on predicting macroscopic response of microcantilevers and nanowire through the microscopic fidelity of molecular interactions. Top-down and bottom-up multiscale schemes inspired by information passage from one scale to the other will be presented. The top-down scheme links atomic contributions from first principles density functional theory (DFT) calculations or classical molecular dynamics/statics (MD) simulations with kinematic constraints imposed by continuum mechanics. The bottom-up scheme performs detailed DFT or MD calculations in a representative volume at the microscopic level and uses this information to solve the desirable macroscopic response with finite element (FE) analysis. Predicted results from both schemes are compared with experimental measurements.

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