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Abstract for an Invited Paper
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First principles molecular dynamics of heterogenous materials

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The development of accurate and efficient computational frameworks to predict multiple properties of heterogeneous systems is crucial to building a robust strategy for the scientific design of novel materials. I will present some progress in developing first principles methods for the calculation of spectroscopic and transport properties of heterogeneous materials, by coupling ab initio molecular dynamics with many body perturbation theory calculations. I will discuss their application to specific systems, e.g. materials for solar energy conversion and defective solids for quantum information applications.