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Multi-Scale modeling and simulations of materials

The current trial-and-error material development methodology is expensive (> $10M) and time consuming (10 to 20 years). Atomistic multi-scale design has the potential to accelerate the material development through the predictive modeling of mechanical properties and corrosion resistance of new materials. The success of atomistic simulations depends critically on its ability to accurately account for chemical reactions, predict mechanical properties and handle large atomic systems within a reasonable time frame. Traditional Quantum Mechanics (QM) approaches are too computationally expensive and, therefore, can handle only very small atomic systems typically at the sub-nano level. This critical issue was successfully addressed in this work by developing, a multi-scale framework with the following components: (i) first-principles Density Functional Theory (DFT) total energy analysis, (ii) Molecular Dynamics (MD) – Monte Carlo (MC) hybrid simulation technique, and (iii) ReaxFF reactive force field scheme that bridges the two. Several case studies will be discussed, which will outline some of the practical applications in solving material problems through the use of multi-scale modeling.

Biography

Alex V. Vasenkov is Senior Principal Scientist at CFDRC. He received his Ph. D. degree in thermophysics and molecular physics from the Russian Academy of Science in 1996. With 15 years of experience, he is an expert in material design, self-assembly processing of nanomaterials, and multi-scale modeling. His research was funded by federal agencies (NSF, DOE, and DoD) and industry (Samsung Advanced Institute of Technology, etc.). He is the co-author of over 30 publications in peer-reviewed journals, 5 patent applications, and book chapter.

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