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First principles atomistic modeling of the strength and mechanical properties of solder alloys

Abstract:

First principles atomistic modeling has progressed to the point of providing reliable and accurate descriptions of materials. These simulations help interpret experimental measurements and can be used to predict the properties of prospective materials that have yet to be fabricated in the lab. In this presentation, I will discuss my group's efforts in using density functional theory (DFT) and ab initio molecular dynamics (AIMD) to calculate the mechanical properties of various solder alloy materials. DFT has been used to study the effect of alloying Bi with various elements on its ductility. AIMD has then been used to reveal how the mechanical properties can change as a function of temperature, which turned out to be useful for predicting the melting point with high reliability. Next, the strength of Cu-Sn solder interfaces is modeled by calculating the energy required to separate the two metals, and how this can be strengthened by substitutional alloying. Finally, I will discuss our group's efforts to implement machine learning and other artificial intelligence techniques to handle more complicated systems such as high-entropy alloys and with large numbers of atoms that cannot be directly handled with first principles techniques.

Bio:

Prof. Smeu obtained his PhD at McGill University in Canada, followed by postdocs at Northwestern University and the Hydro-Québec Research Institute. He joined the faculty at Binghamton University in 2015, where he established a computational modeling lab to study materials for applications in electronics packaging, energy storage, and molecular spintronics with first principles simulations based on density functional theory. In 2024 he was awarded a Humboldt Research Fellowship to carry out sabbatical research at the Helmholtz Institute Ulm in Germany. He has published 67 peer-reviewed articles to date.

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