MM 42 Hauptvortrag Mike Finnis (Max-Born Preisträger)

Zeit: Dienstag 14:00–14:30 Raum: TU H1058

Hauptvortrag MM 42.1 Di 14:00 TU H1058

Atomic size matters — •Mike Finnis — Atomistic Simulation Center, Department of Physics and Astronomy, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, UK — Träger des Max-Born-Preises

"Atomic size" is a concept often referred to by metallurgists when talking about the rules governing the location or behaviour of impurities, but it has been treated with some suspicion by solid-state theorists who do first-principles calculations. I will describe some recent calculations that address a very old problem: why is Cu embrittled by a few tens of parts per million of Bi? There has been some controversy about this kind of effect, with a general belief that it is electronic in origin, whereby the impurity draws electrons from Cu-Cu bonds and weakens them. By means of first-principles calculations we have found [1] that on the contrary, in the case of Bi in Cu the effect can be explained by the larger atomic size of Bi and its insolubility in Cu, and electron transfer appears to be insignificant.

[1] Schweinfest, R., A.T. Paxton and M.W. Finnis, Bismuth embrittlement of copper is an atomic size effect. Nature, 2004. In press.