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Deciphering the vibrational signatures of dopants and defects in random alloys FREE

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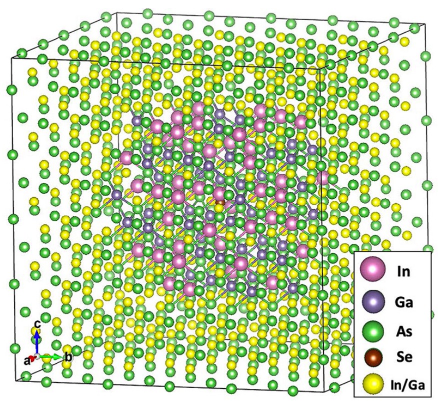
Computational method eliminates background noise and allows researchers to accurately locate dopants and defect species in nanoscale semiconductor devices.



Identifying and locating dopants and defect species in nanoscale semiconductor devices can help optimize their performance. Doing so accurately presents a challenge to researchers, because in random and near-random alloys, it can be hard to gather detailed information about the local environment and species due to background noise in the phonon spectrum.

Jia et al. developed a computational method to identify, or "map," dopants and defect species in semiconductor alloys. Their technique predicts the vibrational signatures, or fingerprints, of the dopants and defects and can be applied to any random alloy. Unlike previous studies on the topic, the authors' calculations take into account multiple local environments for defect sites in random alloys.

"Computational simulations using our method as a map will allow researchers to interpret the phonon spectrum with far less ambiguity in terms of the locations and chemical identities of impurities in any complex alloy material," said author Haili Jia.

The authors tested their approach on a random InGaAs alloy, studying two dopants, silicon and selenium, and a cation vacancy defect. They found their local phonon density of states predictions were in agreement with experimental data.

According to the authors, their technique can help researchers link processing choices to structure and properties, and potentially aid in the future design of tailored materials.

"The natural next step in this research is to develop a more general protocol for the inverse design of complex materials," said author Jingyang Wang.

Source: "Fingerprinting the vibrational signatures of dopants and defects in a fully random alloy: An *ab initio* case study of Si, Se, and vacancies in $In_{0.5}Ga_{0.5}As$," by Haili Jia, Jingyang Wang, and Paulette Clancy, *Journal of Applied Physics* (2020). The article can be accessed at https://doi.org/10.1063/1.5144191.