Anthony Yoshimura
Vincent Meunier
Department of Physics, Applied Physics, and Astronomy,
Rensselaer Polytechnic Institute, 110 8th St, Troy, NY 12180, USA
yoshia@rpi.edu

First principles simulation of local response in transition metal dichalcogenides under electron irradiation

Electron beam irradiation by transmission electron microscopy (TEM) is a common and effective method for post-synthesis defect engineering in two-dimensional transition metal dichalcogenides (TMDs)[1]–[3]. Combining density functional theory (DFT) with relativistic scattering theory, we simulate the generation of such defects in monolayer group-VI TMDs, MoS_2, WS_2, $MoSe_2$, and WSe_2, focusing on two fundamental TEM-induced atomic displacement processes: chalcogen sputtering and vacancy migration. Our calculations show that the activation energies of chalcogen sputtering depend primarily on the chalcogen species, and are smaller for TMDs containing Se. Meanwhile, vacancy migration activation energies hinge on the transition metal species, being smaller in TMDs containing Mo. Incorporating these energies into a relativistic, temperature-dependent cross section, we predict that, with appropriate TEM energies and temperatures, one can induce migrations in all four TMDs without simultaneously producing vacancies at a significant rate. This can allow for controlled manipulation of the TMD crystal for targeted functionality, without the risk of substantial collateral damage.

References

[1] H. P. Komsa, S. Kurasch, O. Lehtinen, U. Kaiser, and A. V. Krasheninnikov, *Phys. Rev. B - Condens. Matter Mater. Phys.*, vol. 88, no. 3 (2013), pp. 1–8.
[2] H. P. Komsa, J. Kotakoski, S. Kurasch, O. Lehtinen, U. Kaiser, and A. V. Krasheninnikov, *Phys. Rev. Lett.*, vol. 109, no. 3 (2012), pp. 1–5, 2012.
[3] W. M. Parkin *et al.*, *ACS Nano*, vol. 10, no. 4 (2016), pp. 4134–4142.

Figure

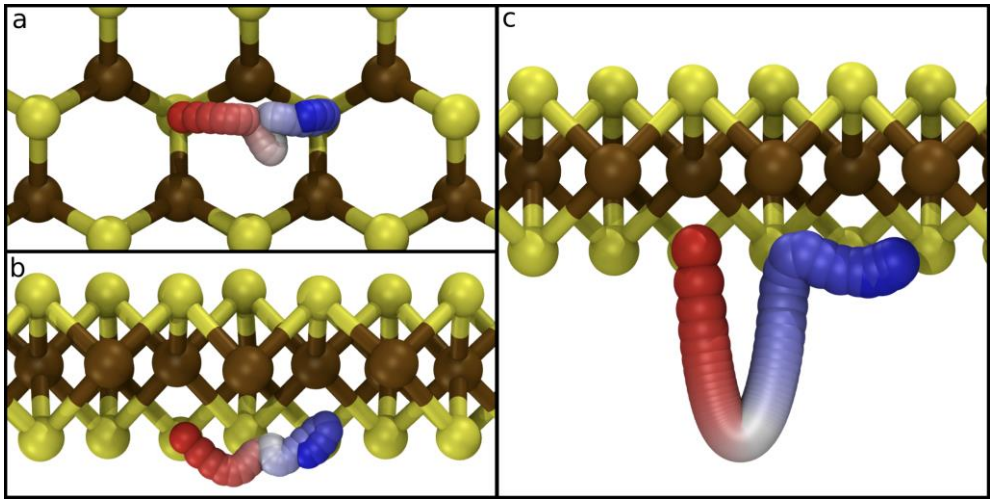

Figure 1: The collision of an incident electron induces the migration of S in MoS_2. (a) and (b) Resulting S trajectory calculated using DFT-based molecular dynamics when 4.10 eV is transferred from the incident electron to the S nucleus

under TEM irradiation of 105 keV. The color gradient from red to blue indicates the time evolution through 300 fs. (c) S trajectory resulting from a more direct collision, with an energy transfer of 7.86 eV. The trajectory runs for 680 fs.