Identifying point defects in liquid-phase exfoliated $PtSe_2$

Ilias. M. Oikonomou[1,2,3], Thomas. Brumme[3], Danielle. Douglas-Henry[1,2], Thomas Heine[3,4] and Valeria Nicolosi[1,2]
[1]CRANN and AMBER, Dublin 2, Ireland
[2]Trinity College Dublin, Dublin 2, Ireland
[3]TU Dresden, Dresden, Germany
[4]Center for Advanced Systems Understanding (CASUS), Görlitz, Germany
oikonomi@tcd.ie

Atom-by-atom characterization of 2D materials is crucial for an in-depth understanding of material properties. Point defects usually degrade the material's performance, but in some cases can induce new properties. $PtSe_2$ belongs to the Noble-Metal Chalcogenides and when it is exfoliated down to a few layers, magnetism has been observed due to the presence of Pt vacancies[1]. Here, we use the low-cost and eco-friendly liquid-phase exfoliation[2] method to exfoliate $PtSe_2$ for energy applications. Aberration-corrected Scanning Transmission Electron Microscopy (STEM), due to its spatial resolution, provides the possibility to observe different kinds of point defects such as vacancies and substitutional defects[3]. However, the interpretation of the results needs validation from STEM imaging simulations. Bloch wave and multislice methods[4], are the two methods that are used for simulating STEM images. Simulated images are compared with experimental images for the quantitative analysis of results. The presence of isolated point defects like Se or Pt vacancies was observed in the exfoliated flakes, as well as more complex defect cases. STEM imaging simulations using the abTEM code and the PRISM algorithm[5] were performed using structures that were fully relaxed within density functional theory. The resulting images were used to train a neural network that can be utilized to accurately and quickly identify complex defects that were observed with low-voltage aberration-corrected STEM imaging.

References

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