Point defect modelling using the Defect Analysis Package (DefAP)

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Key to the development of advanced materials is the ability to predict the concentrations of different defects in any given environmental conditions and how the change in the defect population alters the material's properties. Modern first principles atomistic simulation techniques, such as density functional theory (DFT), are now widely employed for the simulation of point defects, however, to develop true insight into a material's defect chemistry, it is essential to link the energies calculated to thermodynamic variables that fully describe its operating conditions. The Defect Analysis Package (DefAP) [1], an open-source Python code, has been designed to fulfil this role. The primary function of the package is to predict the concentrations of defects in materials as a function of key thermodynamic variables, such as temperature and availability of different species, expressed through chemical potentials. Through simple thermodynamic equations, DefAP allows the rapid exploration of a material's defect chemistry allowing direct comparison with experimental observations.

In this presentation we describe recent developments in the DefAP code and some newly incorporated capabilities, including the ability to incorporate multiple dopants with their own defined concentration, the inclusion of temperature effects into the chemical potentials of reference states and the possibility of predicting the formation of gaseous secondary phases that are poorly defined using DFT. In addition, we demonstrate how DFT and the DefAP package can be combined with neutronics and inventory codes to develop predictive models of how a material's defect chemistry will evolve in a nuclear environment, such as in a fusion reactor [2].

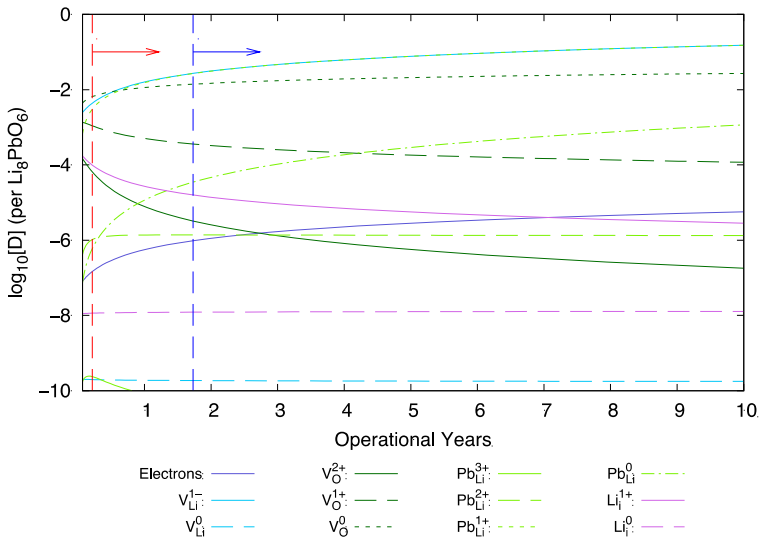

Figure 1: Plot showing the defect chemistry of Li_8PbO_6 as a function of full power operation years in the breeder blanket of a future fusion reactor.

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[1] W. Neilson et.al., "DefAP: A Python code for the analysis of point defects in crystalline solids", Comp. Mater. Sci, 210 111434 (2022).

[2] S T. Murphy et.al., "MODELLING AND DEVELOPMENT OF CERAMICS FOR TRITIUM BREEDING IN FUSION SYSTEMS", IAEA-CN-316/ (2023).