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Calculation of defects and hydrogen in tungsten: fundamental parameters and methodological aspects

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A significant deterioration of tungsten mechanical properties as a result of radiation damage and the accumulation of high concentrations of hydrogen is among the most important problems that are to be solved in order to enable tungsten application in future fusion facilities. The understanding of the defect microstructure development in irradiated tungsten is impossible without knowing the fundamental parameters of primary radiation defects and implanted impurities (first of all - hydrogen). These characteristics include the formation energies of point defects, the solution energies of impurities, defect migration barriers and the energies of interaction between defects. The commonly accepted numerical approach for calculating the parameters of point defects in solids is the density functional theory. However, numerous published DFT studies of point defects in tungsten tend to give remarkably different predictions even for the simplest point defects (for example - for the vacancy formation energy). A possible reason for this situation could be the use of inappropriate or insufficient computational parameters that do not ensure the convergence of calculations results.

This reports describes the results of a detailed systematic study of the influence of the exchange-correlation functional selection, the supercell size, and the technical computational parameters (the cutoff energy and the density of *k*-point mesh in the first Brillouin zone) on the predicted energies of vacancy and interstitial defects, as well as hydrogen atoms in tungsten. We formulate the minimum requirements to the choice of computational parameters that ensure acceptable accuracy of point defect energies. It is shown that calculations in tungsten are very demanding to the choice of parameters, which is more severe than for many other structural and functional materials for fusion reactors and is not satisfied in many already published papers dealing with point defects in tungsten.