Determination of equilibrium concentrations of H and H_2 in Pb melt using *ab initio* metadynamics calculations

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The deployment of fast neutron reactors for closing the nuclear fuel cycle is considered promising for nuclear energy. In these reactors, heavy metal coolants, particularly lead, are used as the primary loop coolant. Hydrogen can enter the primary loop either during cleaning – when hydrogen is introduced into the coolant volume to bind oxygen and dissolve solid-phase PbO oxides – or as part of water molecules in the heat exchange zone between the primary and secondary loops. Since hydrogen actively binds with oxygen, controlling its state in the coolant volume is essential [1].

Ab initio molecular dynamics (MD) calculations allow the study of the behavior of individual atoms and molecules in liquid lead [2]. For our calculations, we use the VASP software package. To determine the thermodynamically equilibrium concentrations of hydrogen atoms and molecules in the lead melt, we calculate the free energy of molecule formation in the melt. The free energy is computed using the metadynamics simulation approach [3], which involves adding an adaptive potential to the MD simulation. For a specific temperature, the thermodynamically equilibrium concentrations of molecular H_2 and atomic H hydrogen impurities in the lead melt is obtained.

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[2] Li D, Zhang Y, He H, Liu C and Pan B 2015 *Journal of Nuclear Materials* **467** 181–185

[3] Bussi G and Laio A 2020 *Nature Reviews Physics* **2** 200–212