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A first principles calculation and statistical mechanics modeling of defects in Al-H system MIN JI, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory-U.S. DOE. and Department of Physics, Iowa State University, Ames, Iowa IA 50011 — The behavior of defects and hydrogen in Al was investigated by first principles calculations and statistical mechanics modeling. The formation energy of different defects in Al+H system such as Al vacancy, H in institution and multiple H in Al vacancy were calculated by first principles method. Defect concentration in thermodynamical equilibrium was studied by total free energy calculation including configuration entropy and defect-defect interaction from low concentration limit to hydride limit. In our grand canonical ensemble model, hydrogen chemical potential under different environment plays an important role in determing the defect concentration and properties in Al-H system.

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