Adsorption and dissociation of high-pressure hydrogen on pipeline steel surface: combining DFT calculation and statistical thermodynamics

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Abstract Hydrogen (H_2) pipeline systems are fundamentally the same as natural gas pipeline networks, but face a more serious safety challenge due to potential hydrogen embrittlement (HE) risk. At present, H_2 transportation and storage are intentionally operated under high-pressure (HP) conditions (*i.e.*, 5-20 MPa for transportation, 35-100 MPa for storage), which make H_2 under supercritical state (*i.e.,* supercritical H_2, s-H_2). In this study, the thermodynamics of H_2 at a wide combination of temperatures (300 - 900 K) and pressures (0.1 - 100 MPa) has firstly been established based on a lattice-molecule model for predicting the adsorption and dissociation of gaseous and supercritical H_2 on the Fe-based steel surface. The configurations of H_2 adsorption and dissociation on Fe (100) and Fe_2O_3 (001) surfaces were investigated through the density functional theory (DFT) calculation, and the corresponding mechanism was elucidated using hybrid orbital theory. By applying the combination of DFT calculation and statistical thermodynamics, the dissociative adsorption of HP H_2 on Fe (100) and Fe_2O_3 (001) surfaces upon varying temperature and pressure was predicted and the results well aligned with previously published experimental studies. Compared to the gaseous H_2, s-H_2 was likely to be more active on the iron (Fe) and its oxide (Fe_2O_3) surface in terms of dissociating into H atoms and could cause steels more susceptible to HE. The results also confirmed that the presence of the Fe_2O_3 scale could protect pipeline steels from environmental hydrogen permeation under the investigated HP conditions.

Keywords: adsorption; dissociation; supercritical hydrogen; high-pressure; pipeline steel