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A QCDFT Study of Hydrogen embrittlement at Crack Tip QING PENG, Rensselaer Polytechnic Institute — Study of hydrogen embrittlement is of great importance due to widespread availability of hydrogen in all environmentally influenced cracking phenomena. We used QCDFT: Density functional theory based Quasi-continuum method to study the system where hydrogen atoms are presented on crack tip surface in single aluminum crystal under mode-I loading. We found that the presence of 0.1% hydrogen atoms increases the energy for nucleation of dislocations and enhance the brittlement of aluminum by 5%. The presence of hydrogen atoms also makes the geometry of crack tip to be sharp. The bonding and electronic charge transfer between hydrogen atoms and aluminum atoms were studied and the mechanism of hydride-induced embrittlement will be discussed.

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