Abstract Submitted
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Hydrogens in Metal Clusters SHUHEI OHNISHI, NEC Fundamental Research and Environmental Research labs. — Atomic and electronic structures of hydrogen atoms in metal clusters are presented by the first principles calculation based on the density functional theory using the linear combination of atomic orbital method. Discussions are focused on a formation of the vacancy-hydrogen cluster at the cluster center mainly in bcc metals. We found characteristic double stable positions at the vacancy site. Electronic structures of double minimum states are studied in terms of the hydrogen induced states. We analyze stabilities of clusters with and without the vacancy typically by the cluster models of $M_{50}H_6$, $M_{50}H_{12}$, and $M_{51}H_6$, respectively (M= Nb, Mo, V, Cr, Fe, .etc.). Cluster size effects and the maximum capacity of hydrogen at the vacancy site will also be discussed.

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