Does Water Adsorb Molecularly or Dissociatively on a Plutonium Surface?\textsuperscript{1} ASOK RAY, RAYMOND ATTA-FYNN, Department of Physics, University of Texas at Arlington — DFT-GGA has been used to study adsorption of water in molecular and dissociative configurations on $\delta$-Pu (111) surface. In molecular state, water is physisorbed in an almost flat-lying orientation at a one-fold coordinated on-top site. The interaction of the water $1b_1$ orbital and the Pu-$6d$ orbital provides the stability of water on the surface, implying that the Pu-$5f$ electrons remain chemically inert. The coadsorption cases of partially dissociated and fully dissociated products at the three-fold hollow sites yield chemisorption, coupled with rumpling of the surface layer and delocalization of the Pu-$5f$ electrons and formation of strong ionic bonds.

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