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Adsorption of Br2 molecule on the Fe/W(110) substrate: Energetics, electronic and magnetic properties

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Using spin-polarized density-functional calculations with generalized gradient approximation (GGA) as the exchange-correlation functional, we report the energetics of adsorption, as well as the electronic and magnetic properties of homonuclear bromine molecule deposited on the Fe/W(110) substrate. The Fe/W(110) substrate consist in Fe monolayer on the topmost W(110) layer such that the Fe atoms are bonded on the bridge adsorption sites of the Wð110Þ surface. Our calculations show that when the Br2 molecule is adsorbed in parallel, oblique or vertical orientation with respect to the surface, the molecule dissociates. However, when the Br2 molecular adsorption is perpendicular to the bridge or top sites, non-dissociative adsorption occurs. We also found that the observed Br2 adsorption properties depend on the interaction between the 4p orbitals of adsorbed bromine specie and the Fe-3d orbitals of Fe atoms of the Fe/W(110) substrate. Furthermore, it is shown that when the bromine atoms are attached on its energetically preferred adsorption sites, the magnetic moments of Fe atoms are reduced while magnetic moment is induced on the bromine atoms. These results are consistent with a previous work on the O2 adsorption.

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