Magnetic properties and Electronic structure of copper adsorbed polar-ZnO surface by density functional calculations

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The II-VI wide band gap compound semiconductor, ZnO, has been extensively investigated for the application to varistor, gas sensor, blue light-emitting diode, and host material of diluted magnetic semiconductors (DMS) due to their unique piezoelectric, electrical, optical, and magnetic properties [1]. Recently, ZnO was intensively investigated as a candidate of DMS host material [2]. It has been reported that 12.5% Cu-doped ZnO shows a half-metallic property and ferromagnetism with a net magnetic moment of 1 μ_B [3], which are desirable characteristics for spintronic devices. During the early stage of spintronic device fabrication, the surface effect could be an important factor to distribute the well-separated Cu dopant atoms not a cluster type on the ZnO-based spintronic devices. Therefore, the adsorption of a Cu adatom on polar-ZnO surface should be intensively studied for physical properties and applicability to devices. In this study, the electronic structure and magnetic properties of Cu adsorbed polar-ZnO surface were investigated through the *ab initio* calculation using projector-augmented-wave (PAW) method. The generalized gradient approximation (GGA) and GGA+*U* methods were employed, as implemented in the Vienna *ab initio* simulation package (VASP) [4]. The total energy of the Cu adsorbed polar-ZnO:p(2×2) surface system was calculated using the surface supercell, consisting of 8 Zn and 8 O slabs with hydrogen atom termination at the bottom layer and a vacuum region of 12.5 Å thicknesses. All atoms in the surface supercell, except for the two bottom layers and hydrogen atoms, were fully relaxed until the remaining force became less than 20 meV/Å. In addition, the spin polarization scheme was applied to the Cu atom to calculate magnetic properties. From the surface formation energy calculation, it was found that the H_3 site was the most stable adsorption site of Cu adsorbed polar-ZnO surfaces with stable ferromagnetism. The Zn-rich ZnO:Cu surface system (H_3 site adsorption) was predicted to have a half-metallic property and stable ferromagnetism of 0.72 μ_B magnetic moment, which is a desirable property for the spintronic device applications.

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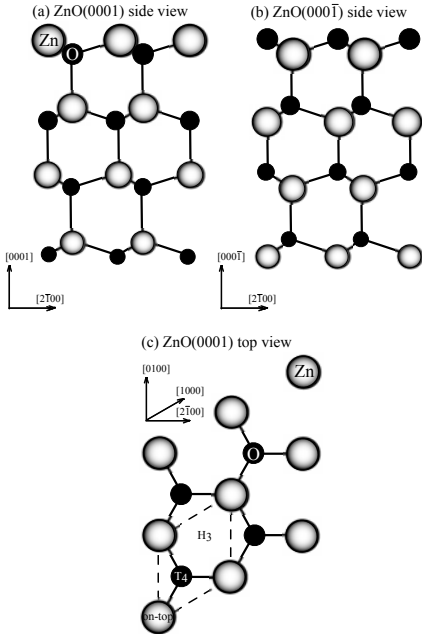

Fig. 1: Schematic illustration of the Wurtzite ZnO surfaces: (a) side view of polar Zn-terminated (0001), (b) side view of O-terminated (000$\bar{1}$), and (c) top view of Zn-terminated (0001) with high-symmetry Cu adsorption sites. The gray circles are Zn atoms and the black circles are O atoms. The surface unit cell is shown by dashed rectangle.

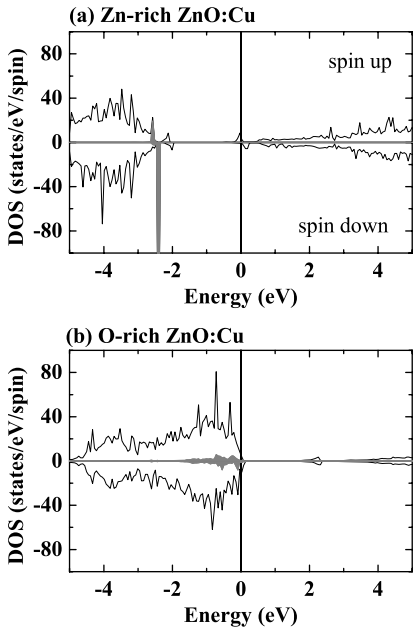

Fig. 2: The total and 3*d*-projected density of states on polar-ZnO:Cu surfaces obtained by the GGA+*U* method. The solid lines represent total density of states and shaded gray regions are 3*d*-projected density of states. The energy of states is referenced to the Fermi level.