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Multiplets in single Fe-phthalocyanine molecule on MgO(001) YUKIE KITAOKA, KOHJI NAKAMURA, TORU AKIYAMA, TOMONORI ITO, Mie University, TOYOKAZU YAMADA, Chiba University — A challenge to miniaturize devices for novel magnetic application now extends to treating the extreme limit of a single atom or molecule. For molecules with transition-metals (TM), multiplet (or electronic configuration) of the d-electrons is an essential aspect in the electronic properties. Further, understandings of molecule-substrate interactions [1] are of crucial importance toward single-molecule-based applications. Previously [2], we demonstrated the utility of the FLAPW method based on the constraint DFT for determining the ground state of the $^3A_{2g}$ electronic configuration in a single FePc molecule. We here address our investigation to treat a single FePc on a MgO(001) substrate. The HOMO and LUMO states, governed by the Fe 3d-orbitals of the FePc molecule, clearly remains in the MgO band gap as seen in the isolated molecule, which gives rise to the ground state of the $^3B_{2g}$ electronic configuration. The transition in the electronic configurations is explained by a weak hybridization between the Fe d_{z2} and O p_z orbitals at the molecule-substrate interface. [1] S. Nakashima et al., Jpn. J. Appl. Phys. **52**, 110115 (2013). [2] K. Nakamura et al., Phys. Rev. B **85**, 235129 (2012).

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