

Abstract Submitted
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Designing the Rashba spin texture by adsorption of inorganic molecules¹ RICO FRIEDRICH, VASILE CACIUC, GUSTAV BIHLMAYER, NICOLAE ATODIRESEI, STEFAN BLÜGEL, Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA — We present an approach in which we show that the spin texture of a surface Rashba system can be adjusted by the adsorption of molecules. By selecting physisorbed and chemisorbed inorganic molecules on the BiAg₂/Ag(111) surface alloy [1] we demonstrate from *ab initio* that both the spin-orbit splitting and the spin direction of Rashba-split surface states can be controlled selectively. The physisorption of NH₃ gives rise to a slightly enhanced outward buckling of the surface Bi which enlarges the magnitude of the Rashba splitting. On the contrary, the weak chemisorption of BH₃ defines a strong inward relaxation of the surface Bi. This causes the occupied Rashba split state to shift into Ag bulk states. In addition a new Rashba splitting is created in an unoccupied state upon BH₃ adsorption. Most importantly, in contrast to the clean surface [1] in case of the BH₃-BiAg₂/Ag(111) system the out-of-plane spin polarization is significantly larger than the in-plane one.

[1] C. R. Ast, *et al.*, PRL **98**, 186807 (2007).

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