Supplementary information for:

Translational Manipulation of Magnetic Cobalt Adatoms on the Si(100)-2x1 Surface at 9 K

*Mayssa Yengui[1,2], Eric Duverger[3], Philippe Sonnet[4] and Damien Riedel[1]**

[1]*Institut des Sciences Moléculaires d'Orsay (ISMO), CNRS, Univ. Paris Sud, Université Paris-Saclay, F-91405 Orsay, France.*

[2]*Laboratoire Matériaux et Génie Industriel, ECAM Rennes – Louis de Broglie, Campus de Ker Lann, Bruz, CS 29128 - 35091 Rennes Cedex 9.*

[3]*Institut FEMTO-ST, Univ. Bourgogne Franche-Comté, CNRS, 15B avenue des Montboucons, F-25030 Besançon, France.*

[4] *Institut de Science des Matériaux de Mulhouse, Université de Haute Alsace, CNRS, IS2M UMR 7361, 3 bis rue Alfred Werner, 68057 Mulhouse, France.*

Corresponding author : damien.riedel@u-psud.fr

Table of contents:

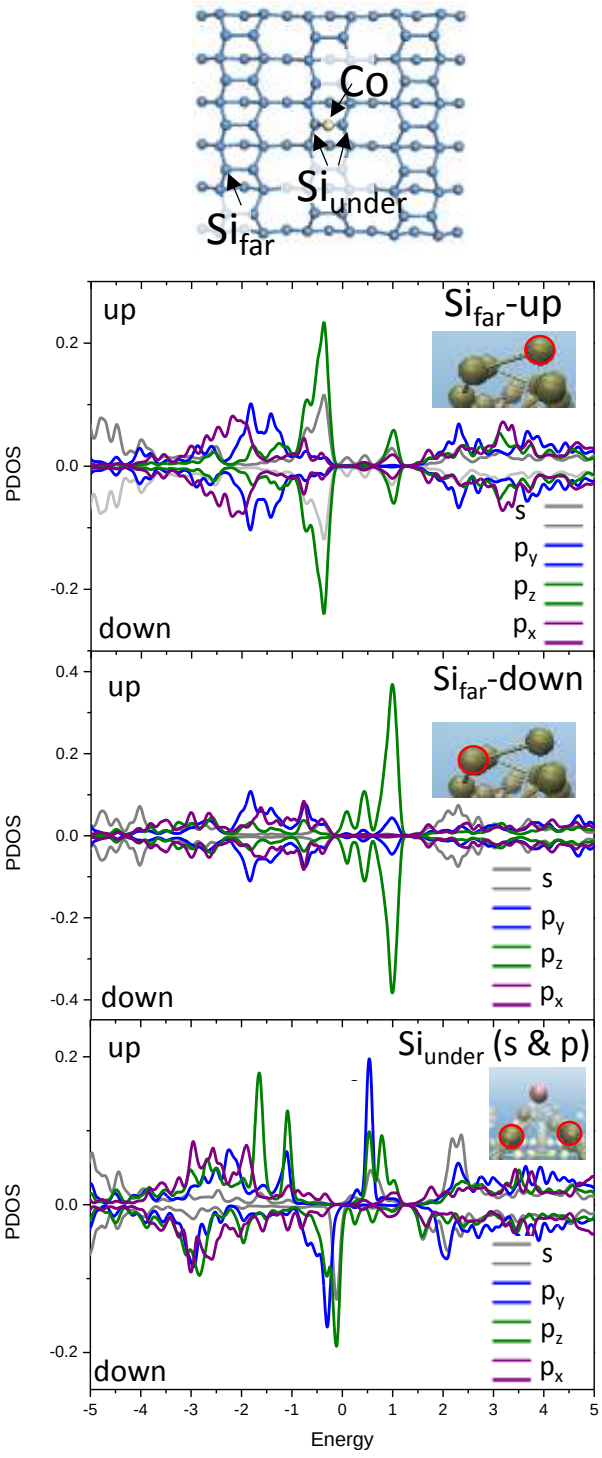

Figure S1: Projected density of states (PDOS) curves calculated on two bare Si atoms located far from the Co adatom and compared with the PDOS on the Si atoms from the dimer located underneath the Co adatom.

The $Si_{far\text{-}up}$ atom exhibits a sharp Si-sp_z hybridization with the neighbor Si atoms and is thus slightly more negatively charged than the $Si_{far\text{-}down}$ atom that sees its net charge being slightly more positive at the Si-p_yp_z empty states.

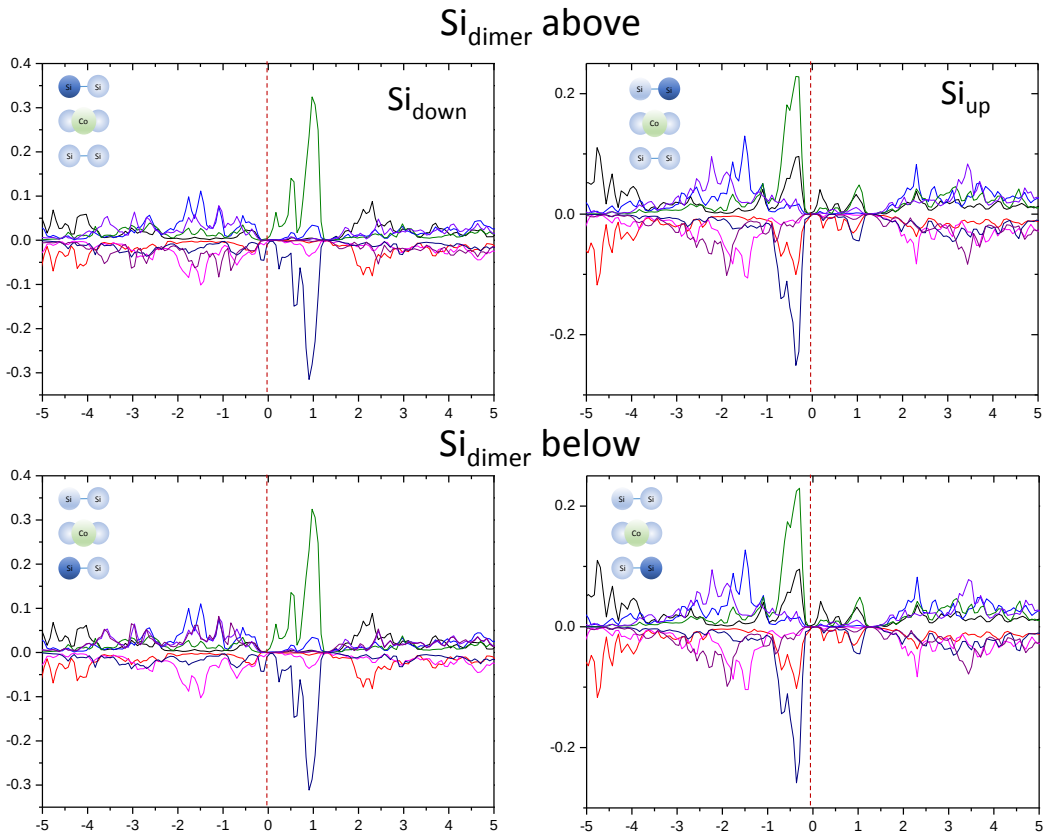

Figure S2: Projected density of states (PDOS) curves calculated on the Si dimers located above and below the Co adatom (without As dopant).

Surface reconstruction	Total energy (eV)	Difference (eV)	Total SMM (μ_B)	Partial SMM from $d_{z^2,yz}$ (μ_B)	Partial SMM from d_{z^2} (μ_B)
p(2x2) with As	-965.147	0.02	1.83	0.43	0.23
c(4x2) with As	-965.127		1.83	0.79	0.26
p(2x2) without As	-965.6390	0.01	1.807	0.45	0.25
c(4x2) without As	-965.6274		1.817	0.71	0.24

Table S1: Evolution of the calculated slab total energy, the total spin magnetic moment (SMM) as well as the partial contribution of the SMM for the orbitals $d_{x^2-y^2}$ and d_{z^2} as a function of the Si(100) surface reconstruction and the presence of As dopant.