Electronic Supplementary Material (ESI) for RSC Advances.

Electronic supplementary information for: Tribochemistry of Phosphorus Additives: Experiments and First-Principles Calculations

M. I. De Barros-Bouchet[1], M.C. Righi[2], D. Philippon[1], S. Mambingo-Doumbe[3], T. Le-Mogne[1], J.M. Martin[1], A. Bouffet[3]

[1] Laboratoire de Tribologie et Dynamique des Systèmes, Ecole Centrale de Lyon - CNRS UMR 5513, F69134 Ecully Cedex France.

[2] CNR Istituto di Nanoscienze Centro S3, Dipartimento di Fisica, Universita' di Modena e Reggio Emilia, 41100 Modena, Italy.

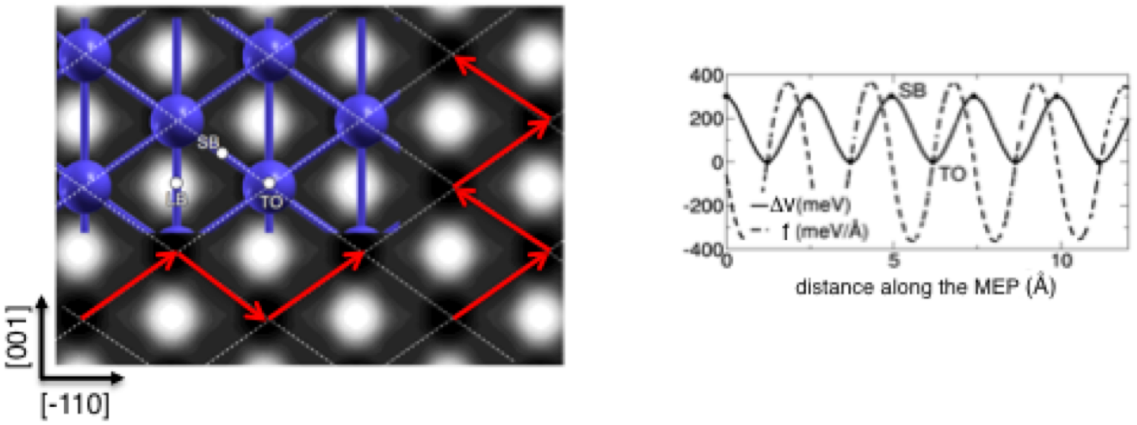
[3] TOTAL, Centre de Recherche de Solaize, 69360 Solaize, France.

Potential energy surfaces of sliding iron interfaces and calculation of shear strength

Two-dimensional representations of the potential energy surfaces (PESes) obtained for the considered interfaces are reported in Fig. 1. In the upper left of each PES a portion of the substrate surface is represented, an identical surface (not shown) should be considered to be sliding quasi-statically on it. For each interface we calculated the interaction potential between the two surfaces at the relative lateral positions indicated by white

circles. In particular, every white circle indicates the position of the LB site of the slider surface (not shown) on the substrate surface (shown). Interpolating the values of the energy obtained for the selected locations we obtained the whole PES, which is displayed in a grayscale representation. The black color is used for the PES absolute minimum and the white color for the PES absolute maximum.

We, then, considered the slider translation along two high symmetry directions indicated by arrows in Fig. 1, namely the [-110] and [001] directions, in the following referred to as the *x* and the *y* directions, respectively. The MEPs followed by the slider when driven along these two directions are indicated in red in Fig. 1. The potential profiles experienced by the slider moving along the MEPs are shown in the graphs on the right side of each PES. The MEPs along the *x* and the *y* directions often coincide. The corresponding lateral forces are obtained as derivatives of the potential and are represented by dashed lines. The maximum restoring force registered for the two considered sliding directions normalized by the cell area are reported in Tab. 1 of the paper .



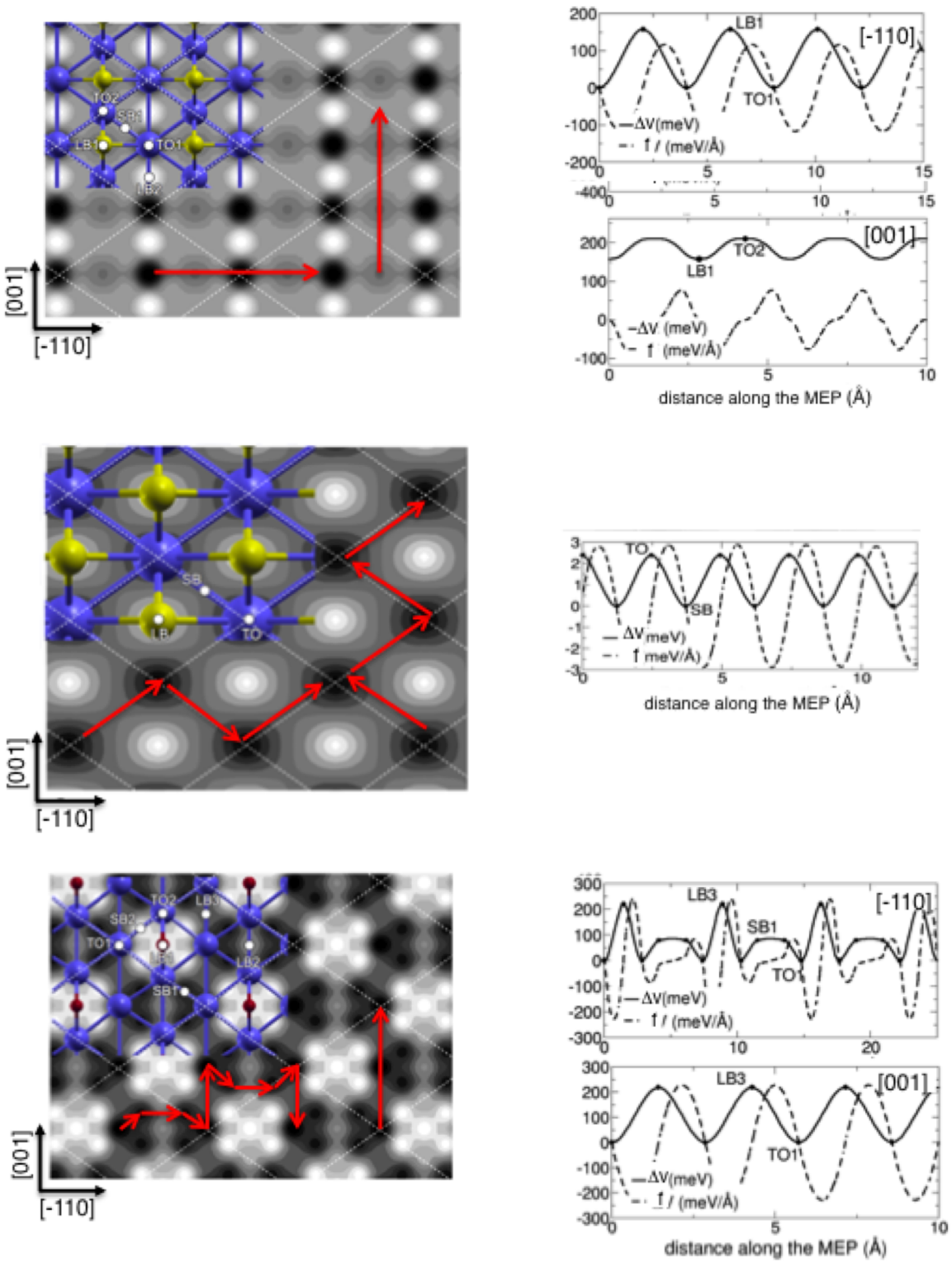


Fig. 1 *Two-dimensional representation of the PESes obtained for the five considered interfaces. Starting from the top: bare interface; phosphorus-terminated interfaces at 0.25 ML, 0.5 ML, 1 ML coverages; oxygen-terminated interface at 0.25 ML coverage. The gray-scale indicates the variation of the surface interaction energy per (1x1) contact with respect to its minimum value. In*

the right panel of each picture the potential profile (full line) and the lateral force (dashed line) per (1x1) contact are plotted as a function of the slider displacement along the MEPs in the [-110] (x) and the [001] (y) directions.