Electronic Supplementary Information
Characterizing Local Metallic Bonding Variation Induced by External Perturbation

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Supplemental Data Items

Fig S1-S7

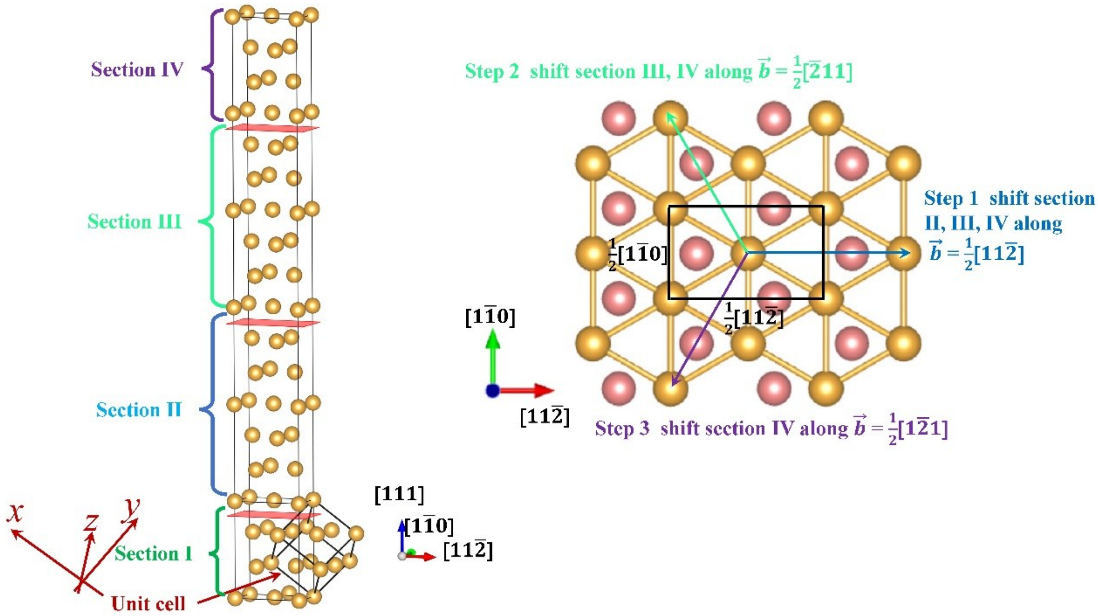

Figure S1. A schematic view of supercell to simulate the generalized stacking fault for fcc metals. The original unit cell and its coordinate frame are shown together with the supercell structure. In order to construct the periodic slab model to accommodate $\frac{1}{2}[11\bar{2}]$ deformation slip, the lattice shift process has to be divided to three steps. In the first step shifting sections II, III and IV relative to section I along $\frac{1}{2}[11\bar{2}]$ direction; next, shifting sections III and IV relative to section II along $\frac{1}{2}[\bar{2}11]$ direction; finally, shifting section IV relative to section III along $\frac{1}{2}[1\bar{2}1]$ direction. Deformation slips along $\frac{1}{2}[11\bar{2}]$, $\frac{1}{2}[\bar{2}11]$, and $\frac{1}{2}[1\bar{2}1]$ directions are symmetry equivalent and possess the same
the generalized stacking fault energy. The total displacement vector of section IV relative to section I is $\frac{1}{2}[11\bar{2}]+\frac{1}{2}[\bar{2}11]+\frac{1}{2}[1\bar{2}1]$ equals to zero, indicating section IV coincides with section I to meet the periodic boundary condition.

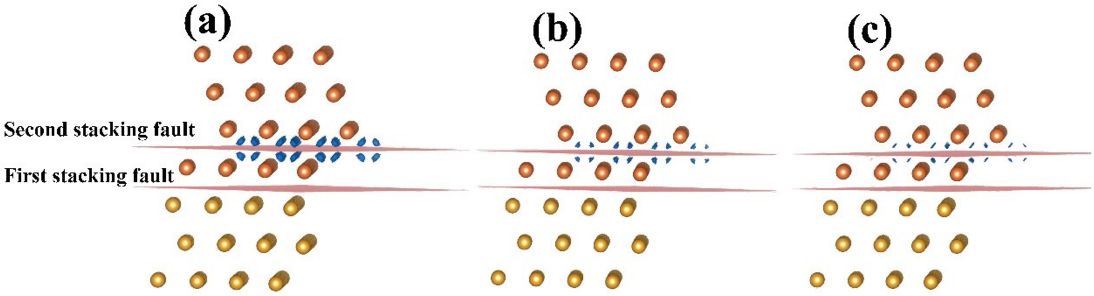

Figure S2. Reduced density gradient on the slip plane for the UST structure of fcc Au at the (a)one-electron charged, (b)neutral, and (c)one-electron deficient states. The plotted isosurface for RDG is 0.085.

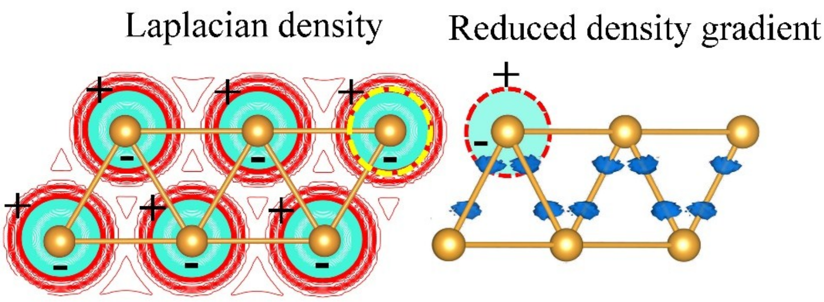

Figure S3. The Laplacian Charge density contour map and reduced density gradient (RDG) for the USF structure of neutral fcc Au surrounding the slip plane. The cyan and red regions represent the negative and positive contour lines respectively. The red circle on the RDG plot is the boundary separating the negative and positive Laplacian Charge densities. The drawn isosurface for RDG is 0.085.

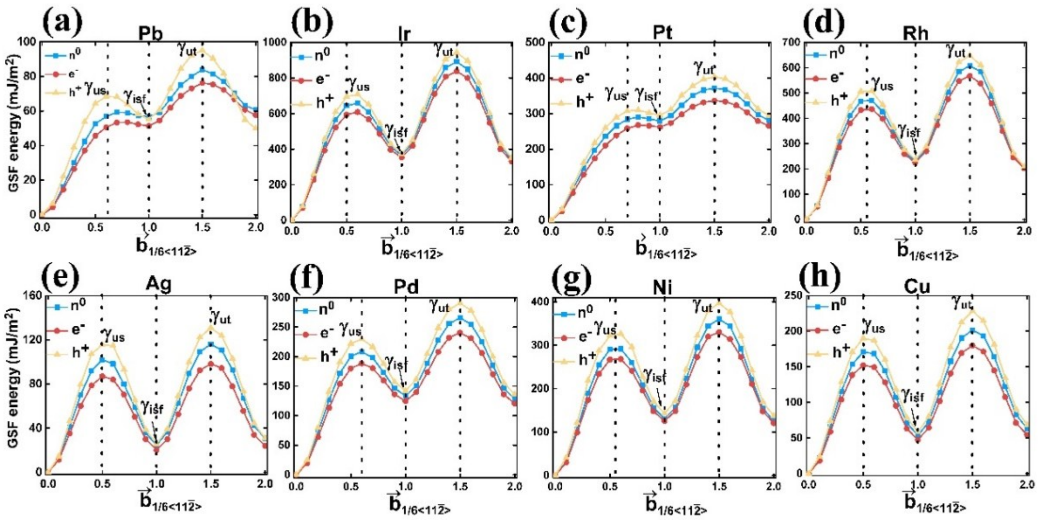

Figure S4. GSFE curves of fcc (a)Pb, (b)Ir, (c)Pt, (d)Rh, (e)Ag, (f)Pd, (g)Ni, and (h)Cu metals with twinning pathways given as a function of the magnitude of the Burgers vector with Shockley partial dislocation $1/6\langle 11\bar{2}\rangle$.

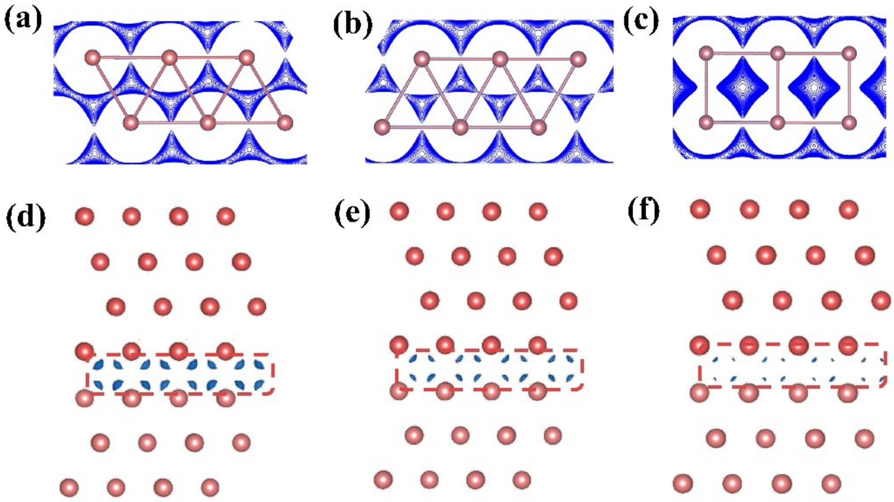

Figure S5. Charge density contour plot for fcc Pb surrounding the slip plane for (a)perfect lattice, (b)USF, and (c)USM structures. Reduced density gradient on the slip plane for the USF structure of fcc Pb at the (d)one-electron charged, (e)neutral, and (f)one-electron deficient states. The drawn isosurface for RDG is 0.085.

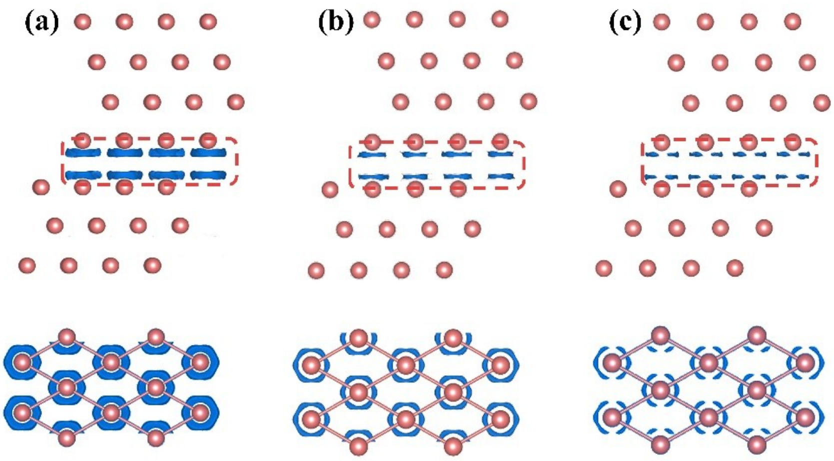

Figure S6. Reduced density gradient on the slip plane for the USM structure of fcc Pb at the (a)one-electron charged, (b)neutral, and (c)one-electron deficient states. The side and top views for the reduced density gradient are shown at the top and bottom. The drawn isosurface for RDG is 0.085.

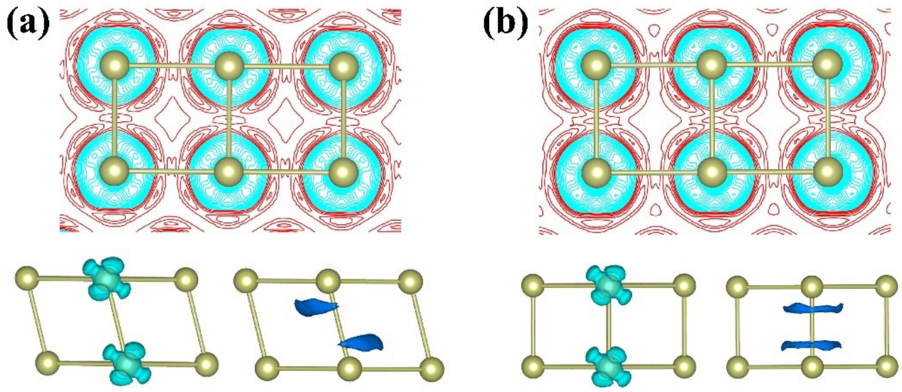

Figure S7. The 2-dimensional Laplacian density, 3-dimensional negative Laplacian density, and reduced density gradient for the deformed fcc Ir structures with maximum energy barrier (a) and with the partial Burgers vector of $2/3a_0\langle 11\bar{2}\rangle$ (b). The cyan and red regions represent the negative and positive isosurfaces of Laplacian density respectively. Reduced density gradient is plotted with the blue isosurface of 0.085.

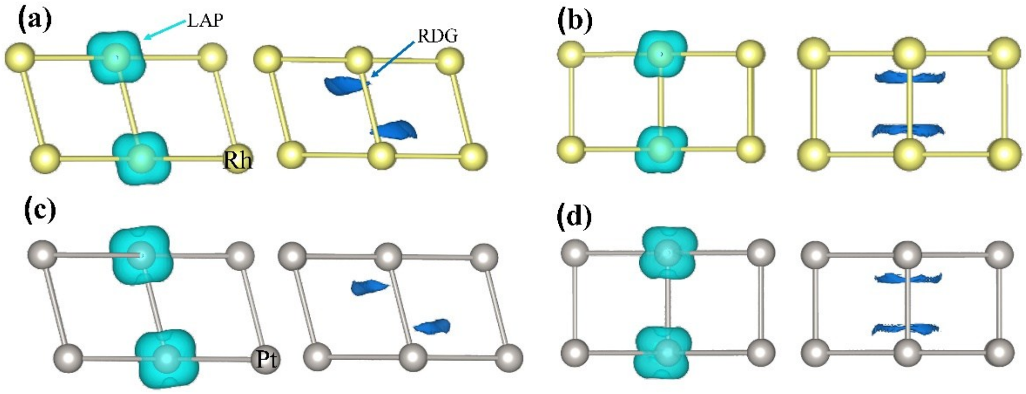

Figure S8. Three-dimensional negative Laplacian density and reduced density gradient (RDG) for the deformed fcc Rh and Pt structures along the fault pathway with (a), (c) the maximum energy barrier and (b), (d) the partial Burgers vector of $2/3a_0\langle 11\bar{2}\rangle$. The cyan isosurface represents the negative Laplacian density. Reduced density gradient is plotted with the blue isosurface of 0.085.