ReadMe

This deposit comprisesg ten folders, split across two compressed archives (Data1 and Data2)…

1. Denominator_Data (in Data1)

This folder contains files pertaining to the calculation of the softness denominator, as defined in the associated paper. File names (*.castep, *.bands, *.odi, *.odo formats, amongst others) reflect the element and facet involved (e.g. Pd111), the size and symmetry of the surface unit cell (e.g. p1x1), the number of slab and vacuum layers (e.g. 26_26), and the charge state (e.g. m0.24). Files processed using our cross correlation code (see next folder description) are provided in *.xcorr format.

2. Cross_Correlation_Code (in Data2)

This folder contains a copy of the Xcorr computer code, which was used to produce the *.xcorr files mentioned in the preceding folder description. The xcorr.readme file provides an explanation of the code's concept, installation, and usage.

3. Geometry_Optimisation (in Data2)

This folder contains geometry optimisation calculations for clean and CO-adsorbed metal surfaces (Cu, Ag, Au, Rh, Pd, Pt). File names (*.castep format) reflect the element and facet involved (e.g. Ag100), the size and symmetry of the surface unit cell (e.g. p1x1), the number of slab and vacuum layers (e.g. 13_13), and the possible presence and disposition of an adsorbate (e.g. CO_upright).

4. Spin_Tests (in Data2)

This folder contains 15 test calculations in which spin was permitted to vary for three different clean palladium surfaces in various charge states. File names (*.castep format) indicate the element and facet involved (e.g. Pd100), the charge states (e.g. negative), and the initial value of the spin parameter (e.g. 1_init).

5. Dispersion_Tests (in Data2)

This folder contains 18 test calculations for the purpose of comparing results with and without Tkatchenko-Scheffler dispersion corrections. File names (*.castep format) indicate the element and facet involved (e.g. Pt110) and the possible presence of an adsorbate (e.g. CO).

6. Planar_Potential (in Data2)

This folder contains electrostatic potentials on a real-space grid (*.pot_fmt format) from calculations for the Pd{100} surface in negative, neutral, and positive charge states. A computer code (planar_plot.f90) is provided that reads this data and produces a planar-average representation as a function of surface-normal grid location (*.out1) or vertical position coordinate (*.out2). The code requires an input file containing key parameters (e.g. grid dimensions) and examples are provided (*.para).

7. Planar_Softneess (in Data2)

This folder contains local softness data on a real-space grid (*.data) calculated for the 18 surfaces discussed in the associated paper. File names reflect the element and facet involved (e.g. Rh110), the size and symmetry of the surface unit cell (e.g. p1x1), and the number of slab and vacuum layers (e.g. 9_9). A computer code (planar_plot.f90) is provided that reads this data and produces a planar-average representation as a function of surface-normal grid location (*.out1) or vertical position coordinate (*.out2). The code requires an input file containing key parameters (e.g. grid dimensions) and examples are provided (*.para).

8. Work_Functions (in Data2)

This folder contains electrostatic potentials on a real-space grid (*.pot_fmt format) from calculations for the Pd{100} surface in negative, neutral, and positive charge states, as calculated in supercells featuring different numbers of vacuum layers (indicated in filenames as vac10, vac12, vac14, and vac16). Together with the Fermi level reported in corresponding *.castep files, the data may be used to calculate work functions as a function of vacuum thickness.

9. Topology_Data (in Data2)

This folder contains calculated local softness on a real-space grid for the 18 surfaces discussed in the associated paper (*.data). File names reflect the element and facet involved (e.g. Ag111), the size and symmetry of the surface unit cell (e.g. p1x1), and the number of slab and vacuum layers (e.g. 8_8). Together with other input files (*.atoms, *.in, *.occupy) these may be analysed via the Topology computer code, provided elsewhere in this archive (see below) to produce atomic softness values for each system (*.out).

10. Topology_Code (in Data2)

This folder contains a copy of the Topology computer code (topology_3.00.f90) used to partition space according to Bader's theory of Atoms in Molecules, and to assign atomic softness accordingly. The file named topology.readme provides an explanation of how to use the code, and includes descriptions of example input files (*.atoms, *.in, *.occupy, and *.zeff).