Development of the ReaxFF Reactive Force-Field Description of Gold Oxides

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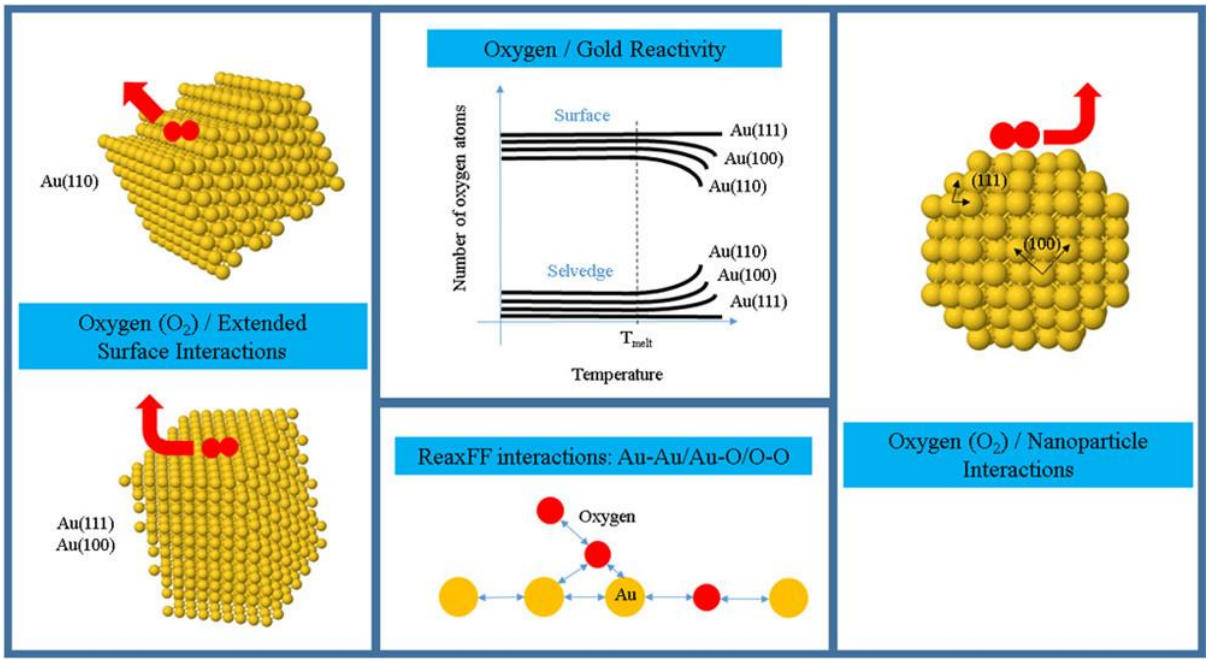
A new reactive force-field (ReaxFF) interatomic potential has been derived for the Au/O system [1]. The potential has been trained across an extensive set of bulk and surface Au and Au/O systems, and describes both the bulk systems and gas-surface interfaces. The potential is shown to be able to simulate the interactions between oxygen molecules and the low-index Au(111), missing-, pairing-row and trench reconstructed Au(110), and the added-row Au(100) facets. Both relativistic and non-relativistic pseudo-potentials were used to generate distinct training sets, and the quantitative differences between the training sets as well as the quantitative and qualitative differences between the predictions of the two derived force-fields are discussed.

The potential has also been shown to predict, in turn, surface and bulk oxide phase formation using both molecular dynamics (MD) and Grand Canonical Monte Carlo (GCMC) simulations. The generic behaviour of the potential is discussed by comparing ReaxFF predictions for the Au/O system presented in this work in the light of recent developments within the field of gold-catalysed surface processes and the behaviour of transition metal surfaces under strain [2].



References:
[1] I. G Shuttleworth, J. Phys. Chem. C **121**, 25255 (2017).
[2] I. G Shuttleworth, Surf. Sci. **661**, 49 (2017).