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Using DFT-based Cluster Expansions to Study Oxygen Adsorption on Platinum and Gold (111) Surfaces SPENCER MILLER, Carnegie Mellon University — We have studied oxygen adsorption on Platinum and Gold (111) surfaces using Density Functional Theory. We have addressed the limitation on the number of configurations we can consider through DFT through the use of two-dimensional cluster expansions on our DFT data, allowing for rapid energy calculations for any arbitrary surface. We have used the cluster expansion to study adsorption properties and phase behavior on the surface including simulated TPD experiments and atomistic thermodynamics phase diagrams which we compare to experimental behavior.

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