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Phase diagram for the adsorption of oxygen and water on Pt(100) and Pt(111)

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HPC content

In this work adsorption energies were calculated, for each adsorption a clean and adsorbed slab was submitted. For each calculation 3 nodes (~72 cores) were used with each submission containing between 20 to 30 atoms. The computational time, using a PBE functional, was 54.6 min/atom with further considerations given to an optB88 functional which required twice the computational time and a SCF iteration increase by a factor of 13. In addition to energy calculations, vibration and nudge elastic band calculations were done with the NEB calculations required to identify a transition state using 10 steps.

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