Supplementary Information for "Support and Oxidation Effects on Subnanometer Palladium Nanoparticles"

Christopher J. Heard,[†] Stefan Vajda,[†,¶] and Roy L. Johnston[*,‡]

Materials Science Division and Nanoscience and Engineering Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, United States, and School of Chemistry, University of Birmingham, Edgbaston, Birmingham, UK, B15 2TT

E-mail: r.l.johnston@bham.ac.uk

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[*]To whom correspondence should be addressed
[†]Materials Science Division and Nanoscience and Engineering Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, United States
[‡]School of Chemistry, University of Birmingham, Edgbaston, Birmingham, UK, B15 2TT
[¶]Department of Chemical and Environmental Engineering, School of Engineering & Applied Science, Yale University, 9 Hillhouse Avenue, New Haven, Connecticut 06520, United States

Table S1: E_d and E_d/atom for MgO (001) bound Pd_4O_x clusters

Cluster composition	Ed/ eV	Ed per Pd atom /eV atom^{-1}
Pd_4	-5.36	-1.34
Pd_4O_1	-5.35	-1.34
Pd_4O_2	-5.37	-1.34
Pd_4O_3	-5.31	-1.33
Pd_4O_4	-5.35	-1.34

Table S2: E_d and E_d/atom for Alumina bound Pd_4O_x clusters

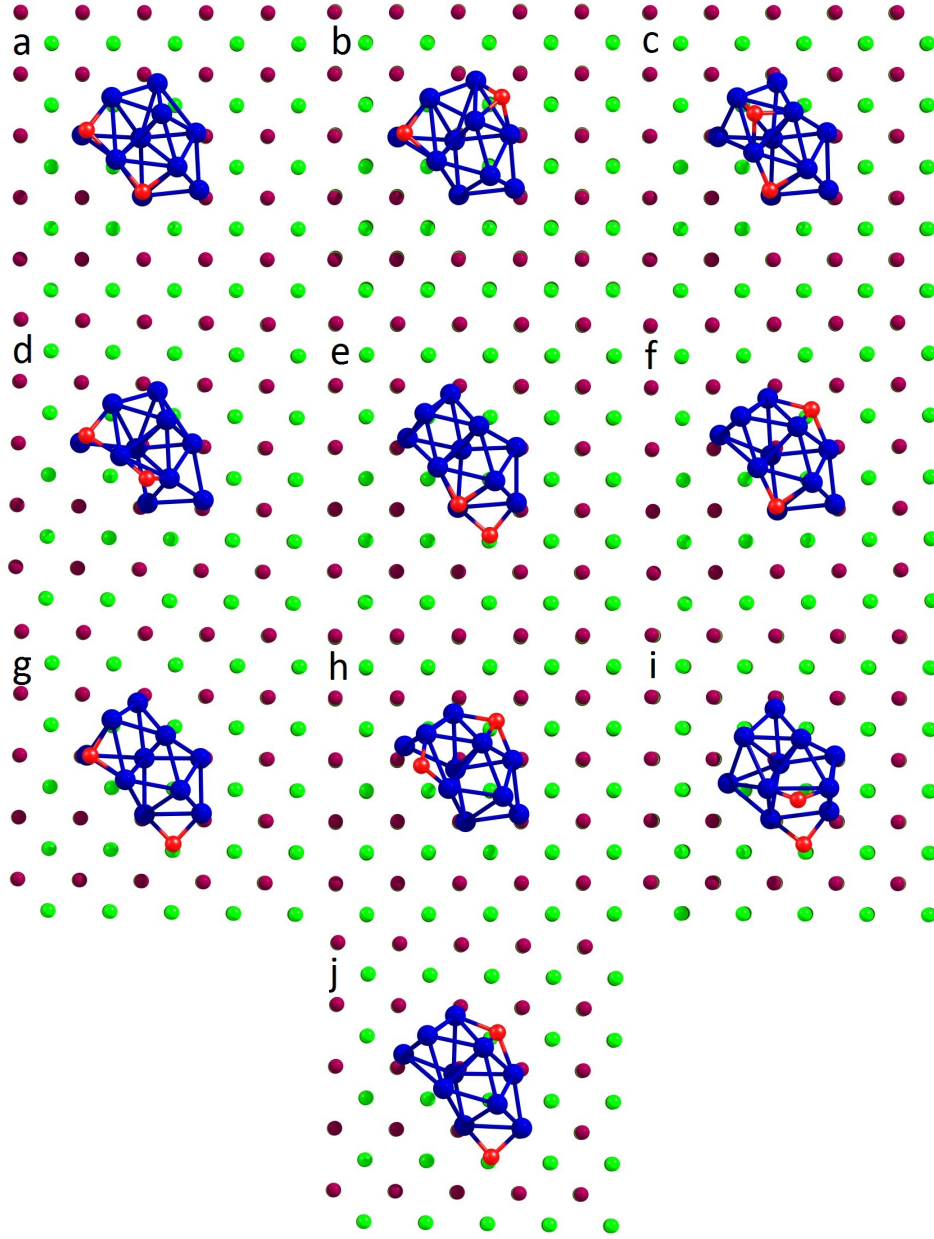| Cluster composition	Ed/ eV	Ed per Pd atom /eV atom^{-1}
Pd_4	-0.20	-0.05
Pd_4O_1	-0.21	-0.05
Pd_4O_2	-0.20	-0.05
Pd_4O_3	-0.15	-0.04
Pd_4O_4	-0.14	-0.04

Figure S3: Candidate structures for $Pd_{10}O_2$ on MgO in order of increasing energy, as given in table 2 in the main text. a) Between layers I, b) Between layers II, c) Between layers + μ-3 top, d) Between layers + μ-2 top, e) Between layers + surf/cluster, f) Between layers II + surf/cluster, g) Between layers III + surf/cluster, h) Surf/cluster + μ-2 top, i) Surf/cluster + μ-2 top, j) Surf/cluster.

Table S4: Bader valence charge transfer to palladium clusters and deposited oxygen atoms for each composition of Pd_4O_x upon MgO. There is a close correspondence between the MgO and Alumina-bound charge transfer, with transfer from the surface to the cluster, and further to the deposited oxygen. The extend of charge abstraction from the surface is larger for MgO than in the Alumina case.

Cluster composition	Pd e^- gain/ e	Oxygen e^- gain /e
Pd_4	0.56	-
Pd_4O_1	-0.20	0.73
Pd_4O_2	-1.05	1.67
Pd_4O_3 (planar)	-2.50	1.76
Pd_4O_3 (3D)	-1.75	2.56
Pd_4O_4	-2.88	3.97