Electronic Suplementary Material for PCCP

Electronic supplemetary information.

Braiding the dynamic threads of structure, function, and reactivity in gas-solid interactions in a single experiment: how Rhodium nanoparticles, of an average 11Å diameter, select for N_2 or N_2O when faced with NO.

Mark A. Newton, Andrew J. Dent, Steven G. Fiddy, Bhrat Jyoti, and John Evans.

Supplementary Table 1: Structural and statistical parameters derived from analysis of the EDE shown in the main paper in EXCURV.

T (K)	Acquisition time (msecs)	k_{min}(Å^{-1})	k_{max}(Å^{-1})	Scatterer	CN	r(Å)	DW($2\sigma^2$)/Å^2	E_F(eV)	R(%)
	Prior to NO exposure, under He								
373	62	3	15,00	Rh	6.7	2.68	0.012	-3,5	43
				Rh		3.70			
				Rh		4.67			
				Rh		5.26			
473	62	2	13,00	Rh	6,35	2,66	0,014	0,5	45
573	62	2	12,00	Rh	5,1	2,63	0,016	0,6	45
647	47	3	11,00	Rh	4,2	2,65	0,024	2,9	80
	After 5%NO/He for 50 secs								
373	62	3	14,00	Rh	3.8	2.70	0.009	-3,4	50
				Rh		3.74			
				Rh		4.70			
				Rh		5.29			
473	62	3	13,00	Rh	3,7	2,68	0,013	-3,7	52
				O	1	2,03	0,012		
				N	0,6	1,77	0,007		
573	62	3	12,00	Rh	1,7	2,65	0,015	1,9	52
				O	1,9	2,06	0,01		
				N	0,8	1,88	0,009		
647	47	3	10,25	Rh	1,6	2,65	0,022	1,6	70
				O	2,4	2,04	0,014		
				N	0,5	1,79	0,012		

Errors in CN should be considered in the range ± 10-20%, those of bondlengths (r) ± 1.5-2%
R(%) = $(\int [\chi^T - \chi^E]k^3dk / [\chi^E] k^3dk) \times 100\%$: χ^T being the theoretically calculated EXAFS and χ^E being the EXAFS obtained via experiment.
σ = the root mean square displacement in interrnuclear separation.

In the simplest aproximation (ref 29, main paper) Rh-Rh first shell co-ordinations of ca. 7 and 4 would indicate Rh nanoparticles of avaerage ca. 40 and 15 atoms respectively.

Similarly bulk Rh_2O_3 would be expected to yield Rh-Rh CN of 2 at ca. 2.71Å and 3O at ca 2-2.1Å.