Supplementary material to:

Structural and Electronic Properties of Nanostructured HAlO

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(Dated: September 10, 2005)

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I. DFT CALCULATIONS

In the parameter-free density-functional calculations we constructed various structures that subsequently were allowed to relax to their closest total-energy minima. The structures as well as the notation we have used in classifying them are all shown in Fig. 1. The results of the density-functional calculations are given in Table I.

TABLE I: Calculated energy and interatomic distances for $[\text{HAlO}]_n$ ($n = 1, 2, 3, 4, 5, 6$). The energy has been corrected for zero-point energy. The distances correspond to mean values where applicable. Indices t and b describe terminal and bridging atoms. Symmetry is given as calculation/final point group.

		Point-	Distances [Å]							
Descriptor	E_{corr} [a.u.]	group	$r(\text{Al-H}_t)$	$r(\text{Al-H}_b)$	$r(\text{Al-O}_t)$	$r(\text{Al-O}_b)$	$r(\text{Al-Al})$	$r(\text{O-O})$	$r(\text{H-H})$	$r(\text{O-H})$
[HAlO] ₁										
aloh	-318.16322	$C_{6v}/C_{\infty v}$				1.6996				0.9677
halo	-318.11333	$C_{6v}/C_{\infty v}$	1.5871		1.6221					
[HAlO] ₂										
lin-mu-o	-636.42522	D_{2h}	1.5849			1.7697	2.4256	2.5776	5.5953	
lin-mu-oh	-636.37530	D_{2h}				1.9306	3.0680	2.3442	4.3011	0.9784
lin-mu-oo	-636.35228	C_{2v}	1.5952		1.6214	1.7075	3.4148	3.3104	2.8383	
al2oh2	-636.33029	C_2				1.7054	3.0782	5.5354	6.8824	0.9694
lin-mu-h	-636.23347	D_{2h}		1.7588	1.6281		2.5993	5.8554	2.3702	
[HAlO] ₃										
ring-mu-o	-954.72562	D_{3d}	1.5851			1.7324	3.0751	2.9199	5.8206	
plane-mu-o	-954.67121	C_s	1.5973			1.8134	2.9355	2.8780	4.7145	
lin-mu-oo	-954.67032	C_1	1.5933			1.7466	3.8840	2.9748	6.4606	
trig-mu-h	-954.58814	C_{2v}	1.5751	1.7739	1.6276	1.9016	2.5652	3.0237	3.7617	
lin-2mu-ho	-954.55361	C_1	1.5806	1.7576	1.6267	1.7683	3.3397	4.5752	4.4134	
al3oh3	-954.51875	C_1				1.7286	2.7300	5.3566	6.5476	0.9755
ring-mu-h	-954.36277	D_{3d}		1.7363	1.6275		3.3488	6.1673	2.4700	
[HAlO] ₄										
cub-mu-o	-1273.05037	T_d	1.5806			1.8749	2.6772	2.6252	5.2583	
ring-mu-o	-1272.98709	D_{4h}	1.5859			1.7178	3.7769	3.3858	6.3294	

TABLE I: (continued)

Descriptor	E_{corr} [a.u.]	Point-group	Distances [$\text{\AA}$]							
			$r(\text{Al-H}_t)$	$r(\text{Al-H}_b)$	$r(\text{Al-O}_t)$	$r(\text{Al-O}_b)$	$r(\text{Al-Al})$	$r(\text{O-O})$	$r(\text{H-H})$	$r(\text{O-H})$
lin-mu-ooo	-1272.91490	C_1	1.5981			1.7348	5.0132	3.5084	8.2092	
lin-mu-oho	-1272.87182	C_1	1.5828	1.7531		1.7633	4.1403	4.3977	5.7720	
al4oh4	-1272.76716	S_4				1.7205	2.6366	5.4417	6.6758	0.9730
ring-mu-ho	-1272.72861	C_{2h}	1.5838	1.7488	1.6271	1.7789	3.8537	4.8416	4.7634	
ring-mu-h	-1272.48132	C_1		1.7370	1.6270		3.9534	6.5720	2.8265	
cub-mu-h	-1272.47012	T_d		1.8777	1.6249		2.9478	5.6012	2.2782	
[HAIO] ₆										
ring2x6-mu-o	-1909.65698	D_{3d}	1.5814			1.8603	3.2486	3.0481	5.6654	
cub+6-ha'	-1909.58188	C_1	1.5825	1.7881		1.8575	3.4577	3.1810	5.6753	
cub+6-hi	-1909.57340	C_s	1.5849			1.8290	3.6694	3.0216	5.3431	
cub+6-ha	-1909.56678	C_s	1.5894			1.8548	3.6021	3.2393	5.3452	
cub+2x2z-hi	-1909.56360	C_1	1.5886			1.8584	3.2685	3.1870	5.6223	
cub+2x2e-hi	-1909.56193	C_{2v}	1.5827			1.8381	3.5053	3.3162	5.7434	
ada+2x1e	-1909.54773	C_1	1.5886	1.7933		1.8362	3.5065	3.1243	5.4868	
ring2x6-4	-1909.54571	C_i	1.5896			1.7784	4.2039	4.0339	6.2067	
cub+6-ha''	-1909.53883	C_s	1.5892			1.8485	3.6943	3.4691	5.9060	
lin-mu-hoooh	-1909.53550	C_1/C_2	1.5842	1.8061		1.8335	3.9707	3.5569	6.2156	
plane-mu-o	-1909.53087	C_i	1.5874			1.8384	4.1983	4.1216	5.9853	
cub+2x2z-ha	-1909.52826	C_2	1.5937			1.8899	3.4395	3.2350	5.6831	
cub+2x2e-ha	-1909.52782	C_{2v}	1.5933			1.8876	3.5428	3.3232	5.4311	
ring2x6-6	-1909.52572	C_s	1.5868			1.8018	3.7007	3.3834	5.9281	
cub2x-ha	-1909.51807	C_1	1.5934			1.8871	3.3077	3.0947	5.5340	
ada+2x2e-hi	-1909.51031	C_1/C_2	1.5849	1.7640		1.7874	3.8175	3.7871	5.4199	
ada+2x2z-hi	-1909.50526	C_1/C_s	1.5852	1.7868		1.7888	3.7455	3.7812	5.2133	
ada+2x1e-ha	-1909.46485	C_1	1.5975	1.7842		1.7905	3.7780	3.1773	5.9154	

TABLE I: (*continued*)

Descriptor	E_{corr} [a.u.]	Point-group	Distances [$\text{\AA}$]							
			$r(\text{Al-H}_t)$	$r(\text{Al-H}_b)$	$r(\text{Al-O}_t)$	$r(\text{Al-O}_b)$	$r(\text{Al-Al})$	$r(\text{O-O})$	$r(\text{H-H})$	$r(\text{O-H})$
ada+2x1z-ha	-1909.46166	C_1	1.5968	1.7800		1.7926	3.7098	3.1794	5.3807	
ada+2x1z-hi1	-1909.45455	C_1	1.5908			1.8502	3.9051	3.1589	5.9548	
ring6+3x2-ha	-1909.44613	C_1	1.6029			1.7605	4.2643	3.9692	6.6531	
ring2x6-mu-ho	-1909.40234	C_3	1.5921			1.8918	3.5211	3.0666	4.2533	0.9809
lin-mu-oohoo	-1909.36173	D_{2h}	1.5977	1.7516		1.7455	6.3873	5.4487	9.0537	
ring2x6-mu-h	-1909.33280	C_1	1.5841	1.8174		1.7394	3.8189	4.4422	4.0385	0.9746
lin-mu-ohoho	-1909.31745	C_1	1.5826	1.7523		1.7676	5.8083	6.0474	6.9560	
plane-mu-h	-1909.26593	C_i	1.5827	1.7633	1.6205	1.7081	5.0841	6.5811	4.0594	
oct-al6oh6	-1909.13194	C_1				1.7321	3.0201	5.5199	6.4369	0.9766
lin-mu-hohoh	-1909.12557	D_{2h}		1.7544	1.6262	1.7663	5.8389	7.0977	5.9834

• = e.g. Al, Al-H, Al-O $\wedge$ = e.g. O, H, OH * = H

FIG. 1: The structures and their notation that were considered in the parameter-free density-functional calculations.