

PdH with External Electric Field

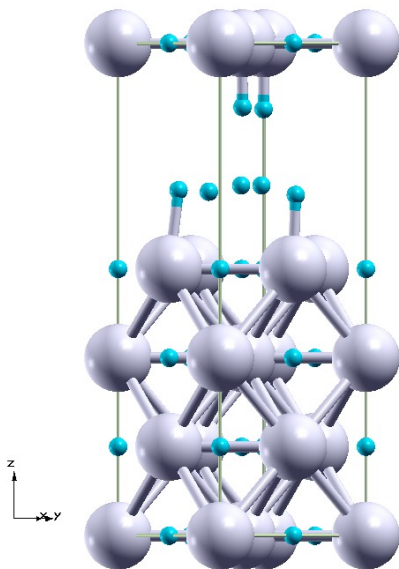
Eunsil Baik

October 3, 2013

Outline

- 1 PdH-3H Triangle
- 2 PdH-4H TSC
- 3 PdH-4H Asymmetry
- 4 PdH Vacancy Simulation

PdH-3H Triangle: Final Geometric Configuration



PdH-3H Triangle: Final Geometric Configuration

$$r = 0.20 \text{ alat} = 0.820 \text{ \AA}$$

E _f = 0.01 a.u. = 5.14 V/nm				
	<i>x_f</i>	<i>y_f</i>	<i>z_f</i>	binding
H1	2.051	0.887	7.807	to ad-H-bottom
H2	1.649	2.427	8.001	no
H3	2.453	2.427	8.000	no

E _f = 0.001 a.u. = 0.514 V/nm				
	<i>x_f</i>	<i>y_f</i>	<i>z_f</i>	binding
H1	2.051	0.804	7.879	to ad-H-bottom
H2	1.623	2.449	8.094	to no
H3	2.051	0.804	7.879	to no

PdH-3H Triangle: Final Geometric Configuration

$$r = 0.21 \text{ alat} = 0.861 \text{ \AA}$$

E _f = 0.01 a.u. = 5.14 V/nm				
	<i>x_f</i>	<i>y_f</i>	<i>z_f</i>	binding
H1	2.051	0.810	7.905	to ad-H-bottom
H2	1.652	2.495	8.281	no
H3	2.450	2.495	8.279	no

E _f = 0.001 a.u. = 0.514 V/nm				
	<i>x_f</i>	<i>y_f</i>	<i>z_f</i>	binding
H1	2.051	0.768	7.935	to ad-H-bottom
H2	1.653	2.446	8.215	to no
H3	2.452	2.446	8.212	to no

PdH-3H Triangle: Final Geometric Configuration

$$r = 0.22 \text{ alat} = 0.902 \text{ \AA}$$

E _f = 0.01 a.u. = 5.14 V/nm				
	<i>x_f</i>	<i>y_f</i>	<i>z_f</i>	binding
H1	2.051	0.822	7.957	to ad-H-bottom
H2	1.654	2.505	8.378	to H3
H3	2.448	2.505	8.377	to H2

E _f = 0.001 a.u. = 0.514 V/nm				
	<i>x_f</i>	<i>y_f</i>	<i>z_f</i>	binding
H1	2.051	0.799	7.921	to ad-H-bottom
H2	1.655	2.480	8.294	to to H3
H3	2.447	2.480	8.293	to to H2

PdH-3H Triangle: Final Geometric Configuration

$$r = 0.23 \text{ alat} = 0.943 \text{ \AA}$$

	$E_f = 0.01 \text{ a.u.} = 5.14 \text{ V/nm}$			
	x_f	y_f	z_f	binding
H1	2.051	1.087	7.808	no
H2	1.633	2.311	7.945	no
H3	2.468	2.311	7.945	no

	$E_f = 0.001 \text{ a.u.} = 0.514 \text{ V/nm}$			
	x_f	y_f	z_f	binding
H1	2.051	1.023	7.895	no
H2	1.661	2.365	8.058	to to H3
H3	2.440	2.365	8.058	to to H2

PdH-3H Triangle: Final Geometric Configuration

$$r = 0.24 \text{ alat} = 0.984 \text{ \AA}$$

E _f = 0.01 a.u. = 5.14 V/nm				
	<i>x_f</i>	<i>y_f</i>	<i>z_f</i>	binding
H1	2.051	0.772	7.882	to ad-H-bottom
H2	1.657	2.499	8.585	to H3
H3	2.445	2.499	8.583	to H2

E _f = 0.001 a.u. = 0.514 V/nm				
	<i>x_f</i>	<i>y_f</i>	<i>z_f</i>	binding
H1	2.051	0.825	8.025	to ad-H-bottom
H2	1.659	2.492	8.471	to to H3
H3	2.443	2.492	8.470	to to H2

PdH-3H Triangle: Final Geometric Configuration

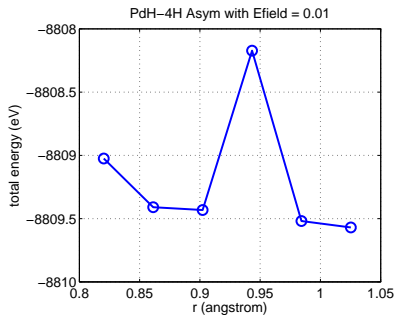
$$r = 0.25 \text{ alat} = 1.025 \text{ \AA}$$

E _f = 0.01 a.u. = 5.14 V/nm				
	x _f	y _f	z _f	binding
H1	2.051	0.772	7.944	to ad-H-bottom
H2	1.657	2.479	8.646	to H3
H3	2.444	2.479	8.644	to H2

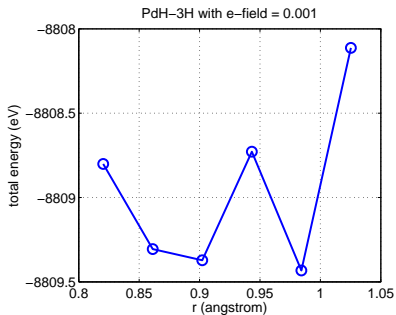
E _f = 0.001 a.u. = 0.514 V/nm				
	x _f	y _f	z _f	binding
H1	2.051	1.117	7.936	no
H2	1.644	2.311	8.080	no
H3	2.457	2.311	8.080	no

PdH-3H Triangle: Energy Comparison

$E_f = 0.01$ a.u. = 5.14 V/nm



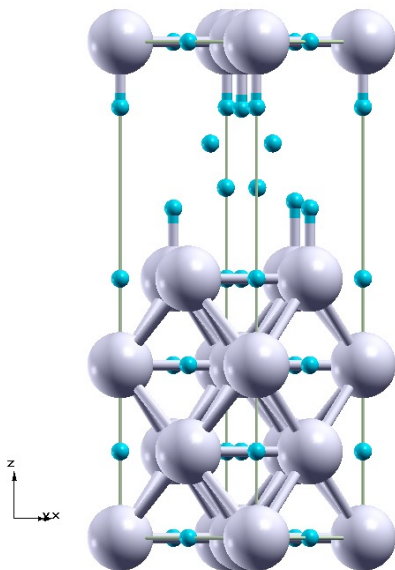
$E_f = 0.001$ a.u. = 0.514 V/nm



Outline

- 1 PdH-3H Triangle
- 2 PdH-4H TSC**
- 3 PdH-4H Asymmetry
- 4 PdH Vacancy Simulation

PdH-4H TSC: Final Geometric Configuration



PdH-4H TSC: Final Geometric Configuration

$$r = 0.20 \text{ alat} = 0.820 \text{ \AA}$$

E _f = 0.01 a.u. = 5.14 V/nm				
	x _f	y _f	z _f	binding
H1	2.051	1.451	8.208	no
H2	2.051	2.651	8.208	no
H3	1.214	2.050	9.159	no
H4	2.887	2.050	9.159	no
d(H12) = 1.200			d(H34) = 1.673	
E _f = 0.001 a.u. = 0.514 V/nm				
	x _f	y _f	z _f	binding
H1	2.050	1.315	7.685	no
H2	2.050	2.796	7.682	no
H3	0.385	2.050	9.458	no
H4	3.721	2.050	9.459	no
d(H12) = 1.481			d(H34) = 3.336	

PdH-4H TSC: Final Geometric Configuration

$$r = 0.21 \text{ alat} = 0.861 \text{ \AA}$$

E _f = 0.01 a.u. = 5.14 V/nm				
	x _f	y _f	z _f	binding
H1	2.051	1.445	8.275	no
H2	2.051	2.656	8.274	no
H3	1.257	2.051	9.177	no
H4	2.844	2.051	9.177	no
d(H12) = 1.211			d(H34) = 1.587	
E _f = 0.001 a.u. = 0.514 V/nm				
	x _f	y _f	z _f	binding
H1	2.050	1.438	8.183	no
H2	2.050	2.664	8.183	no
H3	1.127	2.050	9.152	no
H4	2.974	2.050	9.153	no
d(H12) = 1.226			d(H34) = 1.847	

PdH-4H TSC: Final Geometric Configuration

$$r = 0.22 \text{ alat} = 0.902 \text{ \AA}$$

E _f = 0.01 a.u. = 5.14 V/nm				
	x _f	y _f	z _f	binding
H1	2.051	1.451	8.319	no
H2	2.051	2.650	8.319	no
H3	1.269	2.051	9.248	no
H4	2.833	2.051	9.248	no
d(H12) = 1.199			d(H34) = 1.564	
E _f = 0.001 a.u. = 0.514 V/nm				
	x _f	y _f	z _f	binding
H1	2.051	1.435	8.276	no
H2	2.051	2.666	8.276	no
H3	1.210	2.050	9.188	no
H4	2.892	2.050	9.188	no
d(H12) = 1.231			d(H34) = 1.682	

PdH-4H TSC: Final Geometric Configuration

$$r = 0.23 \text{ alat} = 0.943 \text{ \AA}$$

E _f = 0.01 a.u. = 5.14 V/nm				
	x _f	y _f	z _f	binding
H1	2.051	1.462	8.328	no
H2	2.051	2.640	8.327	no
H3	1.239	2.051	9.356	no
H4	2.863	2.051	9.357	no
d(H12) = 1.178			d(H34) = 1.625	

E _f = 0.001 a.u. = 0.514 V/nm				
	x _f	y _f	z _f	binding
H1	2.050	1.456	8.283	no
H2	2.050	2.645	8.283	no
H3	1.179	2.050	9.303	no
H4	2.922	2.050	9.304	no
d(H12) = 1.189			d(H34) = 1.743	

PdH-4H TSC: Final Geometric Configuration

$$r = 0.24 \text{ alat} = 0.984 \text{ \AA}$$

E _f = 0.01 a.u. = 5.14 V/nm				
	x _f	y _f	z _f	binding
H1	2.051	1.468	8.356	no
H2	2.051	2.633	8.356	no
H3	1.229	2.051	9.421	no
H4	2.872	2.051	9.421	no
d(H12) = 1.165			d(H34) = 1.643	

E _f = 0.001 a.u. = 0.514 V/nm				
	x _f	y _f	z _f	binding
H1	2.050	1.461	8.267	no
H2	2.050	2.641	8.266	no
H3	1.120	2.050	9.381	no
H4	2.981	2.050	9.382	no
d(H12) = 1.180			d(H34) = 1.861	

PdH-4H TSC: Final Geometric Configuration

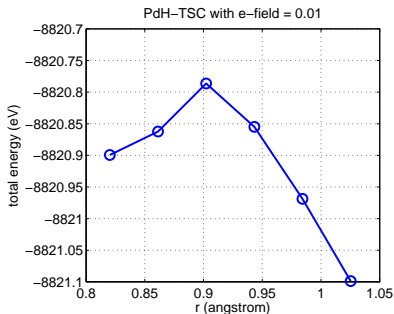
$$r = 0.25 \text{ alat} = 1.025 \text{ \AA}$$

E _f = 0.01 a.u. = 5.14 V/nm				
	x _f	y _f	z _f	binding
H1	2.051	1.455	8.373	no
H2	2.051	2.646	8.373	no
H3	1.200	2.051	9.438	no
H4	2.901	2.051	9.438	no
d(H12) = 1.192			d(H34) = 1.701	

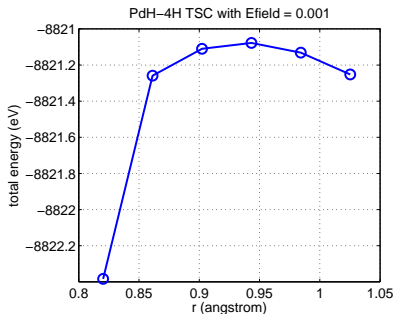
E _f = 0.001 a.u. = 0.514 V/nm				
	x _f	y _f	z _f	binding
H1	2.050	1.444	8.310	no
H2	2.050	2.658	8.309	no
H3	1.113	2.050	9.359	no
H4	2.988	2.050	9.360	no
d(H12) = 1.214			d(H34) = 1.875	

PdH-4H TSC: Energy Comparison

$E_f = 0.01$ a.u. = 5.14 V/nm



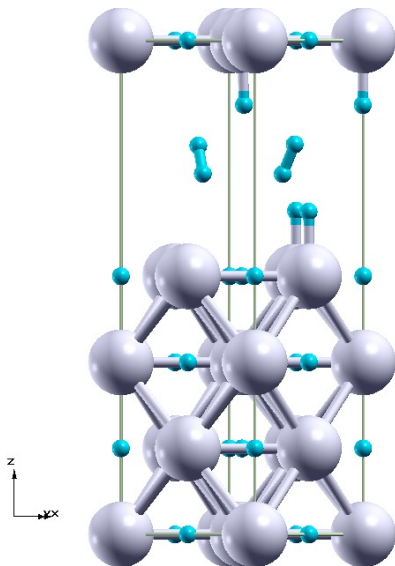
$E_f = 0.001$ a.u. = 0.514 V/nm



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- 1 PdH-3H Triangle
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- 3 PdH-4H Asymmetry**
- 4 PdH Vacancy Simulation

PdH-4H Asymmetry: Final Geometric Configuration



PdH-4H Asymmetry: Final Geometric Configuration

$$r = 0.20 \text{ \AA} \quad a_{\text{lat}} = 0.820 \text{ \AA}$$

E _f = 0.01 a.u. = 5.14 V/nm				
	x _f	y _f	z _f	binding
H1	1.581	1.216	8.386	no
H2	2.497	2.982	8.373	no
H3	1.213	1.412	9.094	no
H4	2.841	3.048	9.191	no
d(H13) = 0.821			d(H24) = 0.890	

E _f = 0.001 a.u. = 0.514 V/nm				
	x _f	y _f	z _f	binding
H1	1.579	1.154	8.335	no
H2	2.526	3.033	8.347	no
H3	1.189	1.396	9.001	no
H4	2.854	3.065	9.074	no
d(H13) = 0.809			d(H34) = 0.799	

PdH-4H Asymmetry: Final Geometric Configuration

$$r = 0.21 \text{ \AA} \quad a_{\text{lat}} = 0.861 \text{ \AA}$$

E _f = 0.01 a.u. = 5.14 V/nm				
	x _f	y _f	z _f	binding
H1	1.519	1.202	8.456	no
H2	2.552	3.014	8.457	no
H3	1.206	1.348	9.222	no
H4	2.848	3.094	9.319	no
d(H13) = 0.840			d(H24) = 0.915	

E _f = 0.001 a.u. = 0.514 V/nm				
	x _f	y _f	z _f	binding
H1	1.628	1.215	8.414	to H3
H2	2.471	2.963	8.415	to H4
H3	1.237	1.461	9.064	to H1
H4	2.815	3.007	9.107	to H2
d(H13) = 0.797			d(H34) = 0.773	

PdH-4H Asymmetry: Final Geometric Configuration

$$r = 0.22 \text{ \AA} \quad a_{\text{lat}} = 0.902 \text{ \AA}$$

E _f = 0.01 a.u. = 5.14 V/nm				
	x _f	y _f	z _f	binding
H1	1.119	1.003	8.759	no
H2	2.859	3.360	8.848	to H4
H3	1.088	0.962	9.561	no
H4	2.966	3.409	9.635	to H2
d(H13) = 0.803			d(H24) = 0.796	

E _f = 0.001 a.u. = 0.514 V/nm				
	x _f	y _f	z _f	binding
H1	1.585	1.196	8.467	no
H2	2.516	2.988	8.481	to H4
H3	1.230	1.413	9.153	no
H4	2.820	3.045	9.187	to H2
d(H13) = 0.802			d(H34) = 0.771	

PdH-4H Asymmetry: Final Geometric Configuration

$$r = 0.23 \text{ \AA} \quad \text{alat} = 0.943 \text{ \AA}$$

E _f = 0.01 a.u. = 5.14 V/nm				
	x _f	y _f	z _f	binding
H1	1.398	1.183	8.837	no
H2	2.653	3.103	8.879	no
H3	1.260	1.259	9.621	no
H4	2.803	3.118	9.672	no
d(H13) = 0.800			d(H24) = 0.807	

E _f = 0.001 a.u. = 0.514 V/nm				
	x _f	y _f	z _f	binding
H1	1.555	1.184	8.524	no
H2	2.545	3.002	8.543	to H4
H3	1.230	1.381	9.230	no
H4	2.824	3.071	9.259	to H2
d(H13) = 0.801			d(H34) = 0.771	

PdH-4H Asymmetry: Final Geometric Configuration

$$r = 0.24 \text{ \AA} \quad a_{\text{lat}} = 0.984 \text{ \AA}$$

E _f = 0.01 a.u. = 5.14 V/nm				
	x _f	y _f	z _f	binding
H1	1.522	1.193	8.609	no
H2	2.570	3.000	8.636	to H4
H3	1.234	1.351	9.358	no
H4	2.821	3.091	9.384	to H2
d(H13) = 0.818			d(H24) = 0.794	

E _f = 0.001 a.u. = 0.514 V/nm				
	x _f	y _f	z _f	binding
H1	1.541	1.160	8.564	to H3
H2	2.563	3.019	8.582	to H4
H3	1.227	1.362	9.267	to H1
H4	2.831	3.090	9.288	to H2
d(H13) = 0.796			d(H34) = 0.759	

PdH-4H Asymmetry: Final Geometric Configuration

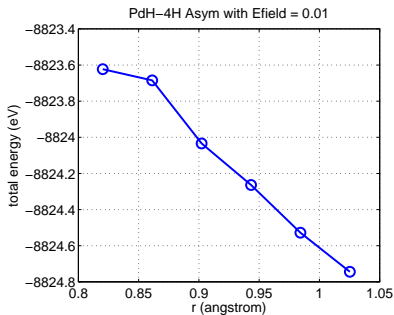
$$r = 0.25 \text{ alat} = 1.025 \text{ \AA}$$

E _f = 0.01 a.u. = 5.14 V/nm				
	x _f	y _f	z _f	binding
H1	1.524	1.169	8.652	no
H2	2.578	3.014	8.672	to H4
H3	1.238	1.348	9.381	no
H4	2.821	3.099	9.391	to H2
d(H13) = 0.803			d(H24) = 0.763	

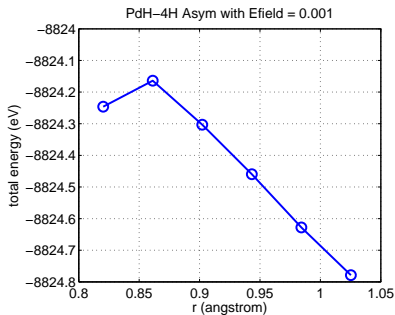
E _f = 0.001 a.u. = 0.514 V/nm				
	x _f	y _f	z _f	binding
H1	1.576	1.154	8.596	to H3
H2	2.522	3.004	8.587	to H4
H3	1.240	1.398	9.266	to H1
H4	2.838	3.068	9.294	to H2
d(H13) = 0.788			d(H34) = 0.777	

PdH-4H Asymmetry: Energy Comparison

$E_f = 0.01$ a.u. = 5.14 V/nm



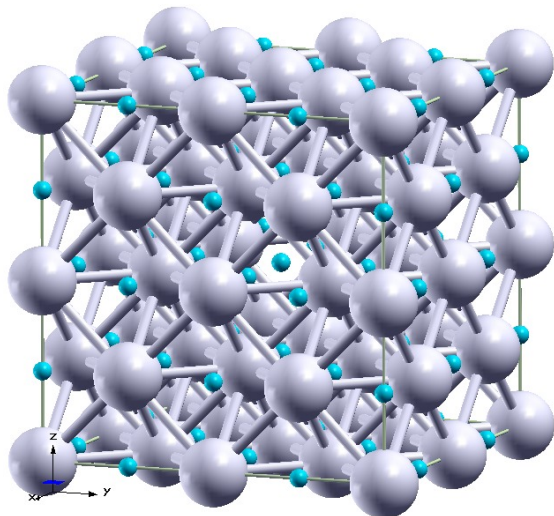
$E_f = 0.001$ a.u. = 0.514 V/nm



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