

Table 1: Sorption energies (eV) for the different possible sites at surface (hollow, bridge, top) and subsurface (octahedral,  $O_h$ , tetrahedral,  $T_d$ ) of Pd(100), Ir(100) and Pd/Ir(100) systems.

(100)	Surface			Subsurface	
	hollow	bridge	top	$O_h$	$T_d$
Pd	-0.456	-0.287	0.230	-0.305	-0.212
Ir	-0.429	-0.431	-0.107	0.221	0.522
Pd/Ir	-0.333	-0.162	0.372	0.061	0.136

Table 2: Sorption energies (eV) for the different possible sites at surface (hollow FCC and HCP, bridge, top) and subsurface (octahedral,  $O_h$ , tetrahedral,  $T_d$ ) of Pd(111), Ir(111) and Pd/Ir(111) systems.

(111)	Surface			Subsurface		
	FCC	HCP	bridge	top	$O_h$	$T_d$
Pd	-0.454	-0.407	-0.306	0.179	-0.338	-0.195
Ir	-0.417	-0.397	-0.325	-0.217	0.162	0.483
Pd/Ir	-0.309	-0.281	-0.163	0.304	-0.080	0.065