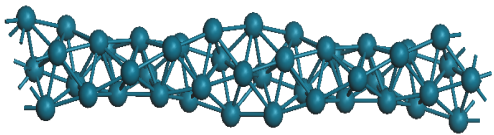
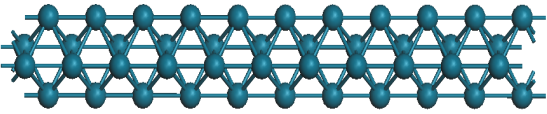
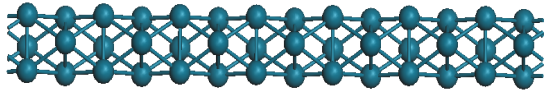


Potential Applications of two ultrathin Pd nanowires to Hydrogen Economy

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Table S-1 The lowest-energy structures and isomers, and binding energy (E_B) (eV) of Pd nanowires

Pd nanowires	E_B (eV)	Structures
	DFT	
1 st (H-wire)	-2.61	
2 nd (O-wire)	-2.60	
3 rd	-2.51	

To find periodic Pd nanowires, the one hundred lowest-energy structures, as determined by SABH calculations, are studied. Three different nanowires with ordered structures were found (see Table S-1). Other nanowires were locally disordered and less stable.