

Supplementary Materials

DFT Investigation of Gas Adsorption and Electronic Modulation on Cd- and Zn-Decorated PdSe₂ Monolayers for Sensor Applications to NO, CO, and NO₂

Achraf Benbella^a, M'hammed Mazroui^a

^a Faculty of Sciences Ben M'Sik, Hassan II University of Casablanca, 20670, Morocco
email address: achraf.benbellaa@gmail.com

Optimized PdSe₂ structure

Number of atoms: 54

Lattice vectors (Å):

```
Lattice="17.265165329 0.0 0.0 0.0 17.702804565 0.0 0.0 0.0 20.000001907"  
Properties=species:S:1:pos:R:3 pbc="T T T"
```

Cartesian coordinates (Å):

Pd	2.87719857	0.00041655	0.81216812
Pd	2.87719807	5.90135069	0.81216790
Pd	2.87719916	11.80228651	0.81216850
Pd	8.63225345	0.00041687	0.81216810
Pd	8.63225333	5.90135110	0.81216796
Pd	8.63225433	11.80228699	0.81216858

Pd	14.38730769	0.00041704	0.81216776
Pd	14.38730743	5.90135129	0.81216762
Pd	14.38730830	11.80228702	0.81216806
Pd	0.00033054	2.95088325	0.81216750
Pd	0.00033103	8.85181711	0.81216716
Pd	0.00033149	14.75275210	0.81216698
Pd	5.75538692	2.95088244	0.81216692
Pd	5.75538756	8.85181660	0.81216656
Pd	5.75538780	14.75275155	0.81216644
Pd	11.51044123	2.95088320	0.81216732
Pd	11.51044201	8.85181706	0.81216696
Pd	11.51044196	14.75275214	0.81216684
Se	0.62606608	0.70585269	0.04932114
Se	0.62606604	6.60678743	0.04932122
Se	0.62606561	12.50772267	0.04932068
Se	6.38112040	0.70585306	0.04932150
Se	6.38112033	6.60678778	0.04932120
Se	6.38111992	12.50772320	0.04932094
Se	12.13617590	0.70585265	0.04932152
Se	12.13617606	6.60678737	0.04932166
Se	12.13617552	12.50772260	0.04932104
Se	5.12881843	5.19904756	1.57614279
Se	5.12881841	11.09998306	1.57614335
Se	5.12881840	17.00091772	1.57614301
Se	10.88387426	5.19904713	1.57614265
Se	10.88387417	11.09998258	1.57614327
Se	10.88387416	17.00091733	1.57614311
Se	16.63892886	5.19904711	1.57614287
Se	16.63892893	11.09998246	1.57614353
Se	16.63892898	17.00091734	1.57614353
Se	3.50376325	2.24857933	1.57614275
Se	3.50376282	8.14951400	1.57614331
Se	3.50376280	14.05044881	1.57614331
Se	9.25881866	2.24857972	1.57614277
Se	9.25881834	8.14951439	1.57614335
Se	9.25881809	14.05044918	1.57614335
Se	15.01387346	2.24857966	1.57614259
Se	15.01387320	8.14951412	1.57614287

Se	15.01387292	14.05044892	1.57614327
Se	2.25146154	3.65632008	0.04932154
Se	2.25146154	9.55725445	0.04932086
Se	2.25146148	15.45818950	0.04932124
Se	8.00651598	3.65631932	0.04932144
Se	8.00651605	9.55725373	0.04932070
Se	8.00651581	15.45818884	0.04932134
Se	13.76157128	3.65631987	0.04932148
Se	13.76157131	9.55725408	0.04932084
Se	13.76157121	15.45818918	0.04932102