

Supplementary Information

Mechanical, thermal transport, electronic and photocatalytic properties of penta-PdPS, -PdPSe and -PdPTe monolayers explored by first-principles calculations

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1- Computational details for optical properties

In the random phase approximation, the imaginary part of the interband dielectric permittivity is given by [1]:

$$\text{Im} \varepsilon_{\alpha\beta}(\omega) = \frac{4\pi^2 e^2}{\Omega} \lim_{q \rightarrow 0} \frac{1}{|q|^2} \sum_{c,v,k} 2w_k \delta(\varepsilon_{ck} - \varepsilon_{vk} - \omega) \times \langle u_{ck+e_\alpha q} | u_{vk} \rangle \langle u_{ck+e_\beta q} | u_{vk} \rangle^* \quad (1)$$

where q is the Bloch vector of the incident wave, w_k is the k-point weight and the band indices c and v are restricted to the conduction and the valence band states, respectively. By using the $\text{Im} \varepsilon_{\alpha\beta}(\omega)$, one can determine the corresponding real part via the Kramers–Kronig relation:

$$\text{Re} \varepsilon_{\alpha\beta}(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\omega' \text{Im} \varepsilon_{\alpha\beta}(\omega')}{(\omega')^2 - \omega^2 + i\eta} d\omega' \quad (2)$$

where P denotes the principle value and η is the complex shift. The adsorption coefficient determined as:

$$a_{\alpha\beta}(\omega) = \frac{2\omega k_{\alpha\beta}(\omega)}{c} \quad (3)$$

where $k_{\alpha\beta}$ is imaginary part of the complex refractive index and c is the speed of light in vacuum, known as the extinction index, given by the following relation:

$$k_{\alpha\beta}(\omega) = \sqrt{\frac{|\varepsilon_{\alpha\beta}(\omega) - \text{Re} \varepsilon_{\alpha\beta}(\omega)|}{2}} \quad (4)$$

The reflectivity is described by:

$$R_{ij}(\omega) = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \quad (5)$$

where n and k are real and imaginary parts of the complex refractive index, which are known as the refractive index and the extinction index, respectively.

2- Atomic structures in VASP POSCAR format

PdPS

```
1.0000000000000000
  5.6901255339477377    0.0000000000000000    0.0000000000000000
  0.0000000000000000    5.7225312188106354    0.0003146491320652
  0.0000000000000000    0.0010996412387334    20.0000999999999998
  P      Pd      S
  4      4      4
Direct
0.8688536317072248    0.7195983874681176    0.4273073849567766
0.8688536317072248    0.7804016125841642    0.3166892096932230
0.1311463832687352    0.2195983874506879    0.4273073849567766
0.1311463832687352    0.2804016125667417    0.3166892096932230
0.7502624153310151    0.1594204594204669    0.2963150729743518
0.7502624153310151    0.3405795405969556    0.4476814773256521
0.2497376145333305    0.8405795106398131    0.4476814773256521
0.2497376145333305    0.6594204892382010    0.2963150729743518
0.3627426258482345    0.4547204925221067    0.4767041966139445
0.6372574040161112    0.9547204925395363    0.4767041966139445
0.3627426258482345    0.0452794961677156    0.2672923758860506
0.6372574040161112    0.5452795073384706    0.2672923758860506
```

PdPSe

```
1.0000000000000000
  5.8420404764721852    0.0000057313269604    0.0003158045741170
  0.0000058325399377    5.8988560743563569    0.0060438911986157
  0.0010816316632133    0.0205103252828701    20.0000000000000000
  P      Pd      Se
  4      4      4
Direct
0.8619892623136423    0.6986709339369952    0.4265941993766305
0.8620441335768732    0.7692779437197856    0.3174008954809864
0.1104022293499014    0.1986718385472415    0.4265956991690203
0.1104571006131323    0.2692788483300319    0.3174023952733691
0.7434902286535561    0.1378005584985402    0.2969226814593924
0.7434162630365933    0.3301508978534855    0.4470718109314689
0.2289561487513652    0.8301491947546111    0.4470738688406115
0.2290301143683351    0.6377989132587416    0.2969247393685350
0.3502700730668451    0.4447438396034684    0.4822610968603911
0.6220782373035973    0.9447450805156308    0.4822575114511949
0.3503681401013310    0.0232046907868479    0.2617390610488002
0.6221763043380832    0.5232059424948758    0.2617354756396040
```

PdPTe

1.0000000000000000

6.0665874203144519	0.0000040488968616	0.0006064123053049
0.0000044497697522	6.1745853926294592	0.0191226716802628
0.0020030579362554	0.0620730110846848	19.9852912972216785

P	Pd	Te
4	4	4

Direct

0.8712532604300378	0.6950797370968900	0.4260445271288731
0.8713468696433040	0.7728690940120799	0.3179497652499919
0.1010994932834706	0.1950806882549401	0.4260468294000077
0.1011931024967367	0.2728700451701371	0.3179520675211265
0.7506656043089066	0.1289263443649986	0.2978488058354998
0.7505393255456383	0.3390255153080517	0.4461440139703896
0.2217807730960217	0.8390234088881527	0.4461477444645041
0.2219070518592900	0.6289242958041754	0.2978525363296143
0.3520569605185457	0.4559744257703287	0.4873458164709845
0.6202137064640567	0.9559755953210143	0.4873417645312870
0.3522326709408716	0.0119741759814644	0.2566548079687081
0.6203894168863826	0.5119753563280156	0.2566507560290106