# SUPPLEMENTARY MATERIAL

**Semiconductor Two-dimensional PdQ2 (Q=S, Se) monolayer: Strain Modulating electronic band gaps and SQ Efficiencies**

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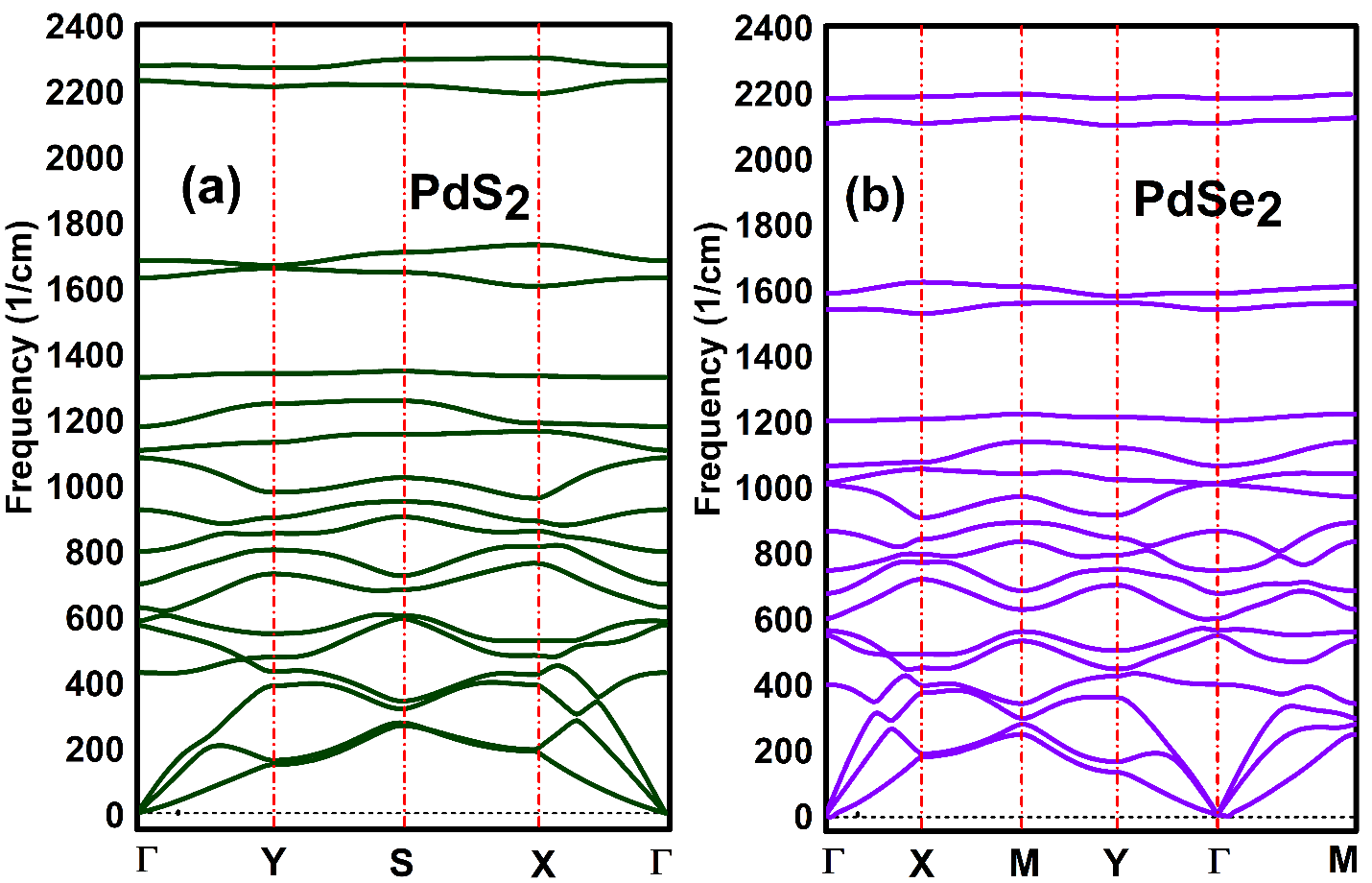
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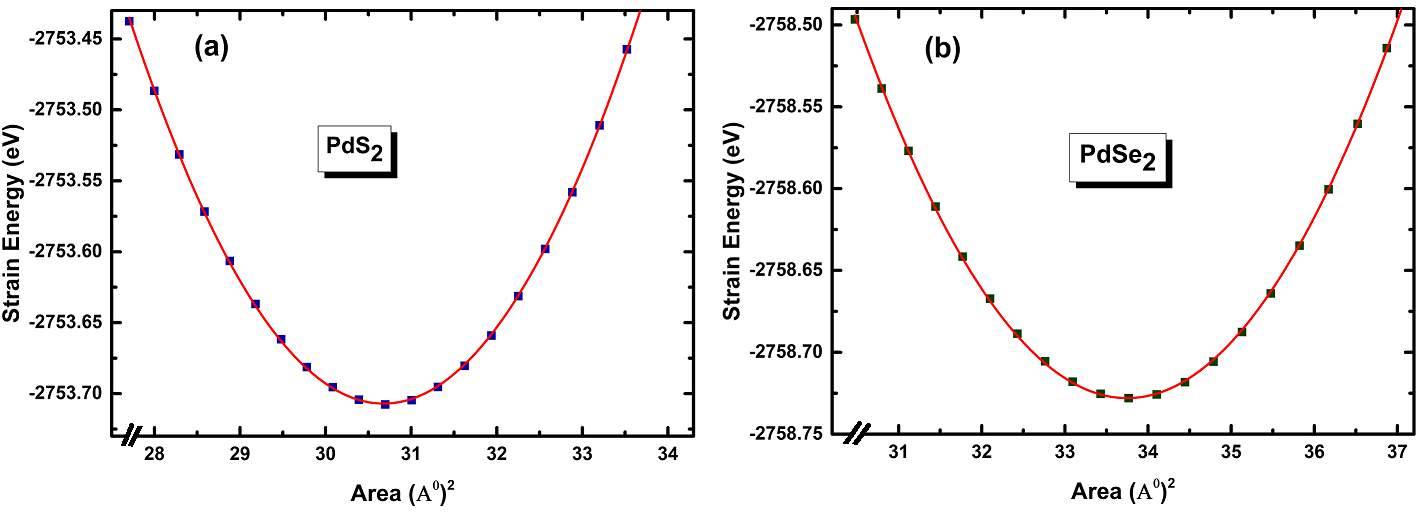
*(24, November, 2021)*

**Keyword (s):** 2D monolayer, Density functional theory, Band structure, Carrier mobility, SQ efficiency

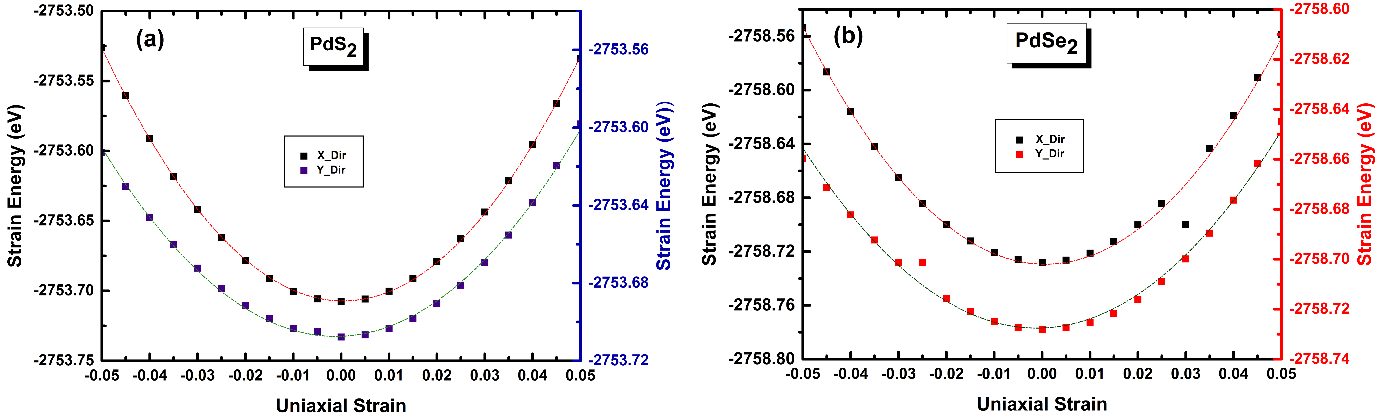
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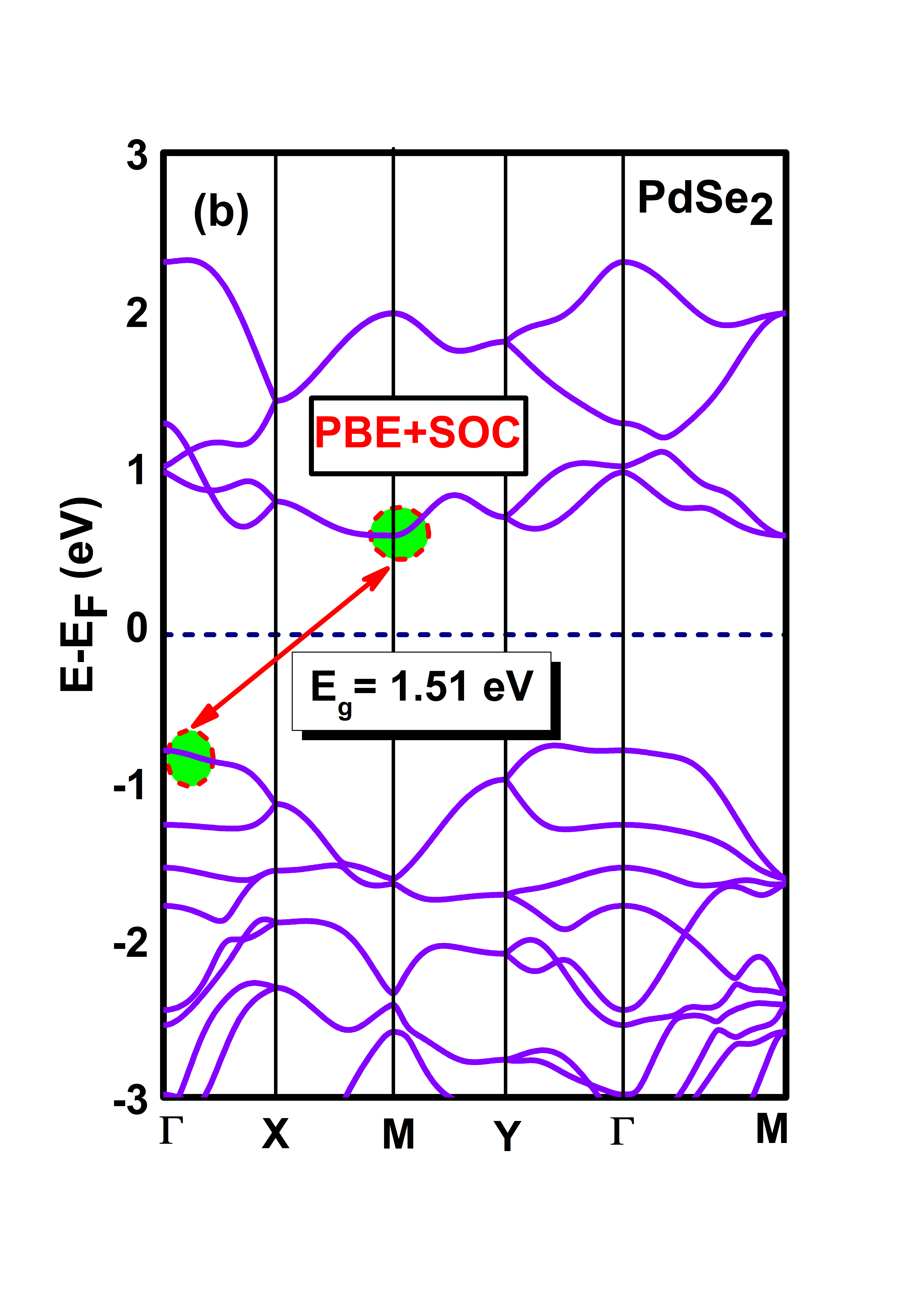
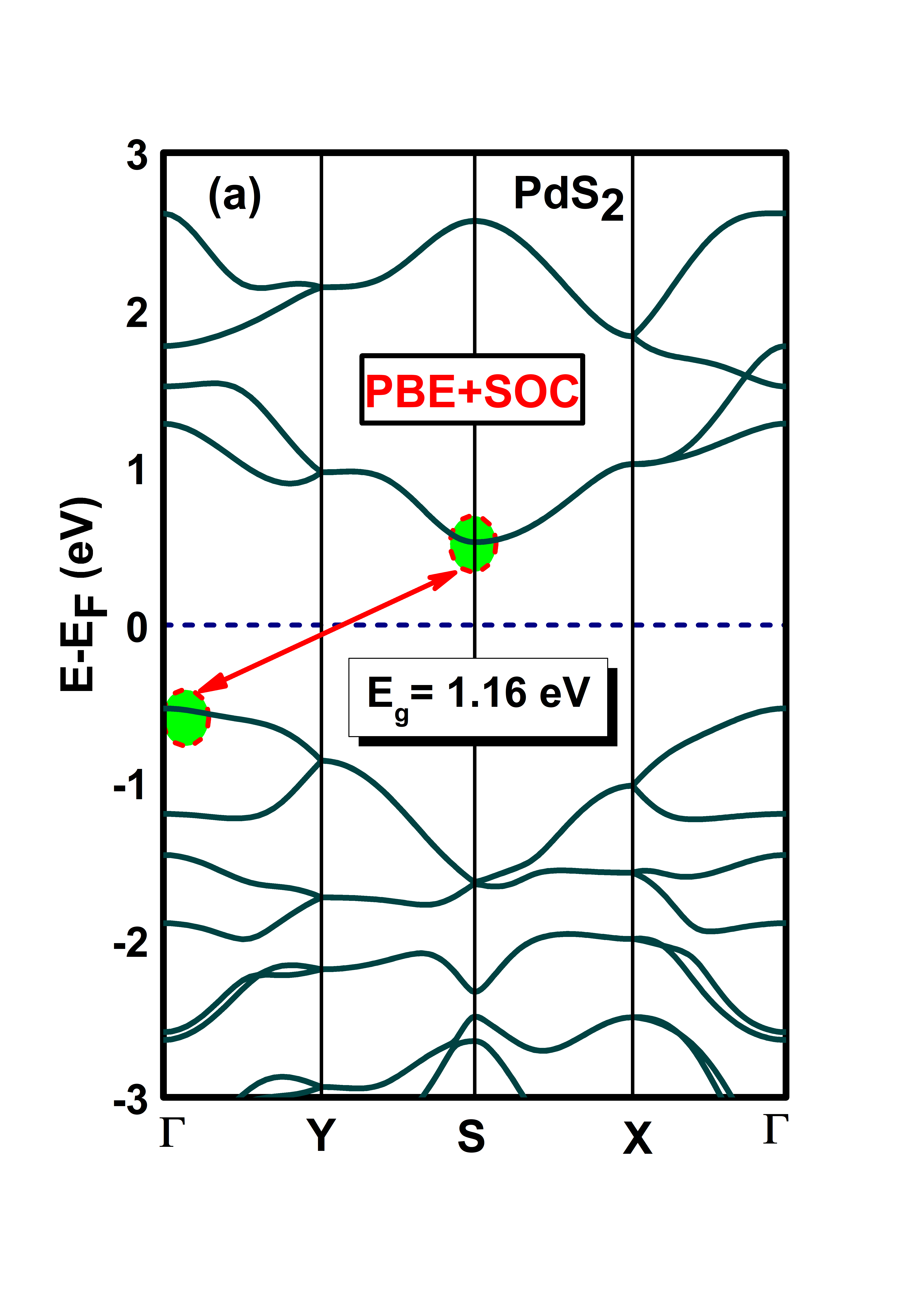
**Figure S1.** (colour online) Phonon spectrum of penta-PdQ2 monolayers. (a) For penta-PdS2 and (b) For penta-PdSe2.



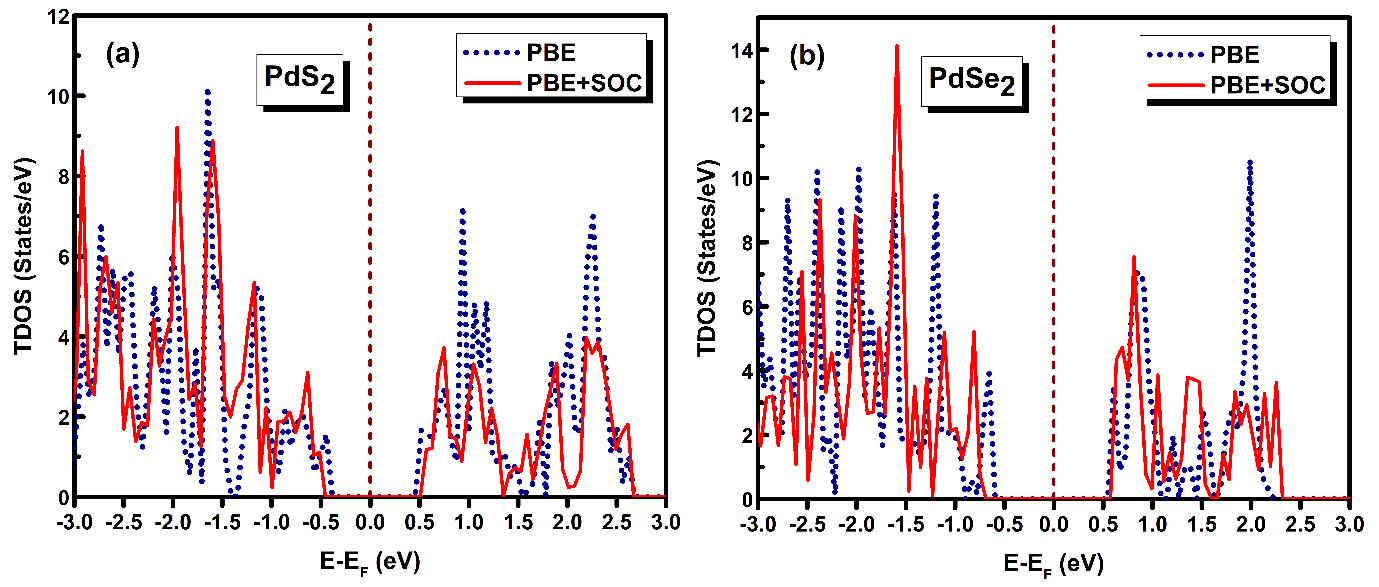
**Figure S2.** (colour online) The Strain energy (eV) vs area (Å2) curve under unstrained and loaded structures. (a) For penta-PdS2 and (b) For penta-PdSe2



**Figure S3.** (colour online) The strain energy (eV) vs uniaxial strain (x or y) curve under pristine and loaded structures. (a) For penta-PdS2 and (b) For penta-PdSe2



**Figure S4.** (Colour online) Electronic band structure of 2D-penta-PdQ2 with PBE+SOC. (a) For penta-PdS2 monolayer and (b) For penta-PdSe2 monolayer.



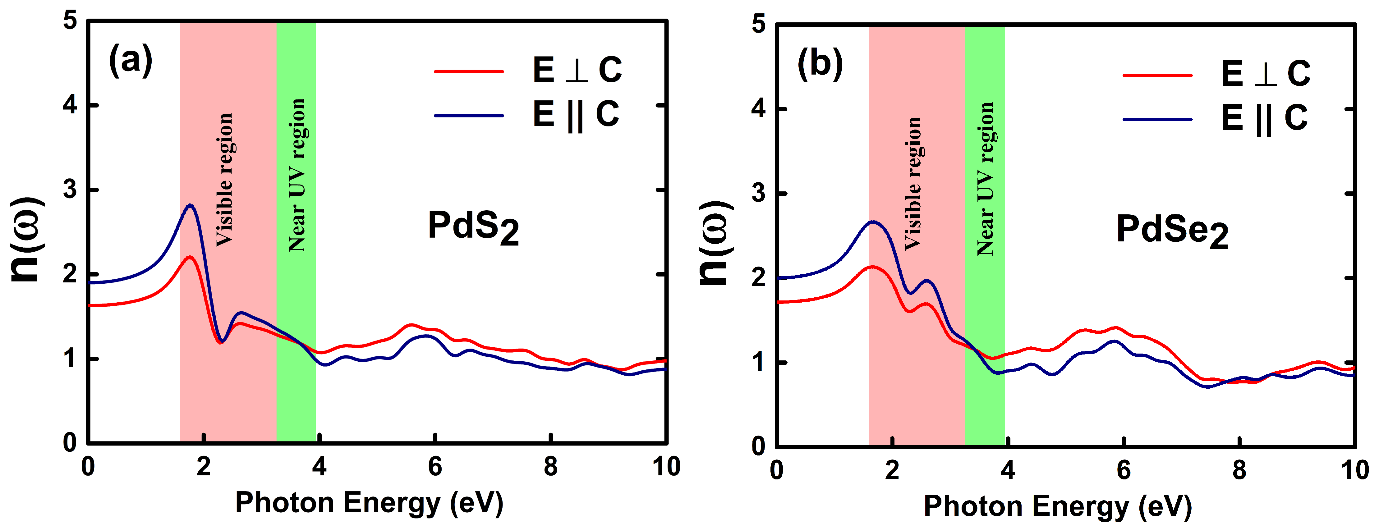
**Figure S5.** (Colour online) Total density of states (TDOS) States/eV with PBE and PBE+SOC calculations. (a) For penta-PdS2 monolayer and (b) For penta-PdSe2 monolayer.

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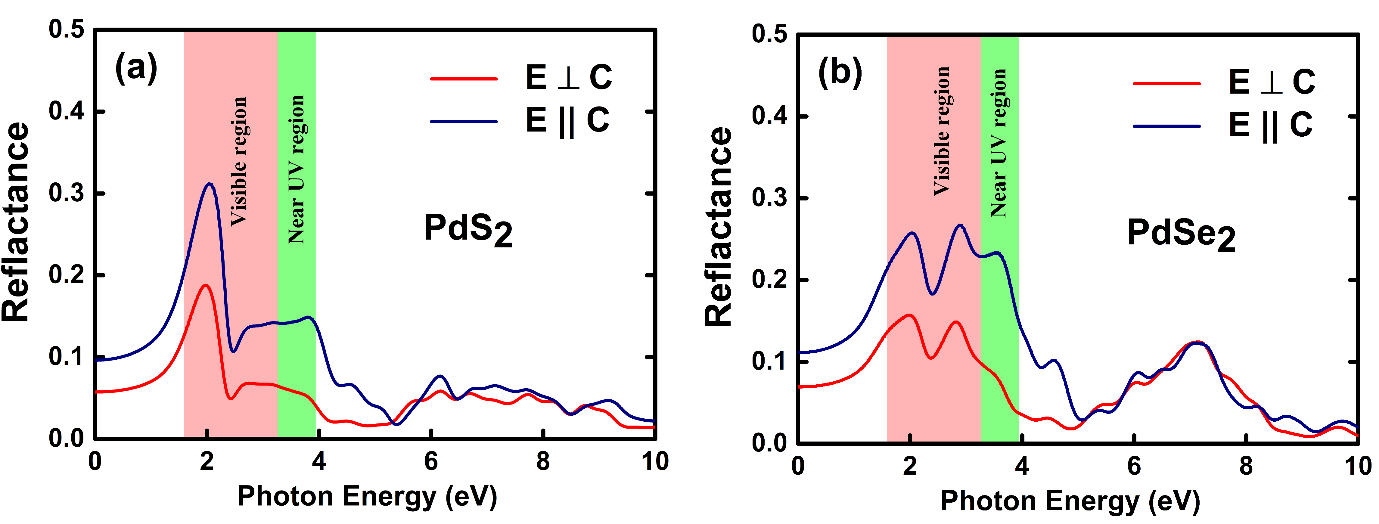
**Figure S6.** (Colour online) Electronic band structure and total density of states (TDOS) States/eV. (a) For penta-PdS2 monolayer under critical tensile strain (+7%) and (b) For penta-PdS2 monolayer under compressive strain (-13%).

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**Figure S7.** (Colour online) Electronic band structure and total density of states (TDOS) States/eV. (a) For penta-PdSe2 monolayer under critical tensile strain (+9%) and (b) For penta-PdSe2 monolayer under critical compressive strain (-13%).



**Figure S8.** (Colour online) Refractive index of penta-PdQ2 monolayers for parallel and perpendicular polarization. (a) For penta-PdS2 monolayer and (b) For penta-PdSe2 monolayer.



**Figure S9.** (Colour online) Reflectance of penta-PdQ2 monolayer for parallel and perpendicular polarization. (a) For penta-PdS2 monolayer and (b) For penta-PdSe2 monolayer.

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| **Penta-PdS2 Monolayer** | | | | **Penta-PdSe2 Monolayer** | | | |
| Compressive strain %  (-Ve) | | Tensile strain % (+Ve) | | Compressive strain % (-Ve) | | Tensile strain % (+Ve) | |
| -13 % | -345.00 cm-1 | -- | -- | -13 % | -1110 cm-1 | -- | -- |
| -12 % | -123.81 cm-1 | -- | -- | -12 % | -1635 cm-1 | -- | -- |
| -11 % | -62.14 cm-1 | -- | -- | -11 % | -76.71 cm-1 | -- | -- |
| -10 % | -56.78 cm-1 | -- | -- | -10 % | -89.43 cm-1 | -- | -- |
| -9 % | -7.35 cm-1 | -- | -- | -9 % | -78.63 cm-1 | +9 % | -23.11 cm-1 |
| -8 % | -2.30 cm-1 | -- | -- | -8 % | -63.03 cm-1 | +8 % | -6.0 cm-1 |
| -7.0 % | -57.47 cm-1 | +7.0 % | Positive Frequency | -7.0 % | Positive Freq. | +7 % | Positive  Frequency |
| -6.0 % | -8.05 cm-1 | +6.0 % | Positive Frequency | -6.0 % | -65.78 cm-1 | +6 % | -12.2 cm-1 |
| -5.0 % | Positive  Freq. | +5.0 % | Positive Frequency | -5.0 % | -65.13 cm-1 | +5.0 % | -40.49 cm-1 |
| -4.0 % | -23.15 cm-1 | +4.0 % | Positive Frequency | -4.0 % | -37.65 cm-1 | +4.0 % | Positive Frequency |
| -3.0 % | -48.68 cm-1 | +3.0 % | Positive  Frequency | -3.0 % | -32.52 cm-1 | +3.0 % | Positive  Frequency |
| -2.0 % | Positive Freq. | +2.0 % | Positive  Frequency | -2.0 % | -35.62 cm-1 | +2.0 % | -7.50 cm-1 |
| -1.0 % | Positive Freq. | +1.0 % | -61.84 cm-1 | -1.0 % | -50.80 cm-1 | +1.0 % | Positive  Frequency |

**Table S1**. Phonon frequencies (cm-1) at Γ-point for different Compressive (-Ve) and tensile (+Ve) strain % on 2D penta-PdQ2 monolayers.