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## Supplementary Information: On The Lubricity of Transition Metal Dichalcogenides: an *ab initio* Study

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Figure 1: Plane-average charge density for the commensurate  $MoS_2$  bilayer at [L] dy = 0.00 Å (global energy minimum) and [R] dy = 3.68 Å (global energy maximum).



Figure 2: Plane-average charge density for the commensurate  $MoSe_2$  bilayer at [L] dy = 0.00 Å (global energy minimum) and [R] dy = 3.84 Å (global energy maximum).



Figure 3: Plane-average charge density for the commensurate  $MoTe_2$  bilayer at [L] dy = 0.00 Å (global energy minimum) and [R] dy = 4.08 Å (global energy maximum).



Figure 4: Charge density difference isosurfaces (isolevel 6.5 x 10E-05 e/A<sup>3</sup>, positive = orange; negative = turquoise) for WSe<sub>2</sub> [L] at dy = 0.00 Å (global energy minimum) and [R] dy = 3.84 Å (global energy maximum)



Figure 5: Plane-average charge density for the commensurate  $WS_2$  bilayer at [L] dy = 0.00 Å (global energy minimum) and [R] dy = 3.68 Å (global energy maximum).



Figure 6: Plane-average charge density for the commensurate  $WSe_2$  bilayer at [L] dy = 0.00 Å (global energy minimum) and [R] dy = 3.84 Å (global energy maximum).



Figure 7: Plane-average charge density for the commensurate  $WTe_2$  bilayer at [L] dy = 0.00 Å (global energy minimum) and [R] dy = 4.08 Å (global energy maximum).



Figure 8: Planar averaged charge density for  $MoS_2$  bilayer, mismatch angle 17.9 degrees, global energy minimum (dy = 7.62 Å)



Figure 9: Planar averaged charge density for  $MoS_2$  bilayer, mismatch angle 17.9 degrees, global energy maximum (dy = 0.00 Å)



Figure 10: Planar averaged charge density for  $MoS_2$  bilayer, mismatch angle 92.2 degrees, global energy minimum (dy = 0.00 Å)



Figure 11: Planar averaged charge density for  $MoS_2$  bilayer, mismatch angle 92.2 degrees, global energy maximum (dy = 13.20 Å)



Figure 12: Plot of the change in potential energy against the integral of the charge accumulated at the interface, for each  $MX_2$  bilayer. The correlation between the two parameters for each bilayer stoichiometry emphasises the finding that greater negative charge accumulation at the bilayer interface is consistent with a lower energy configuration.