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 $6.5 \times 10^{-05} e/A^3$, positive = orange; negative = turquoise) for WSe$_2$ [L] at $dy = 0.00 \text{ Å}$ (global energy minimum) and [R] $dy = 3.84 \text{ Å}$ (global energy maximum)
Figure 5: Plane-average charge density for the commensurate WS$_2$ bilayer at [L] $d_y = 0.00$ Å (global energy minimum) and [R] $d_y = 3.68$ Å (global energy maximum).
Figure 6: Plane-average charge density for the commensurate WSe$_2$ bilayer at [L] $d_y = 0.00$ Å (global energy minimum) and [R] $d_y = 3.84$ 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.