

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

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DATE

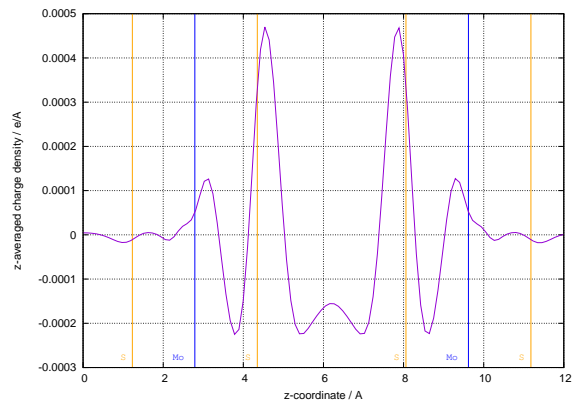
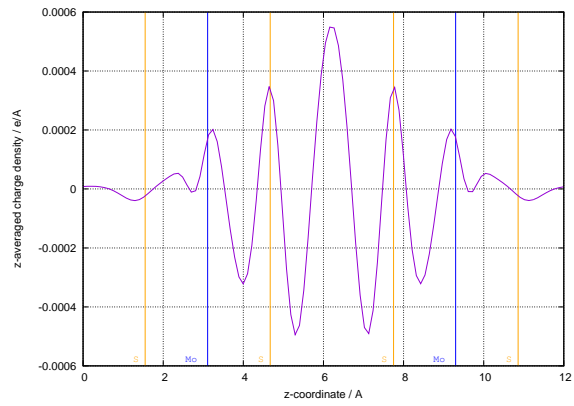


Figure 1: Plane-average charge density for the commensurate MoS₂ bilayer at [L] $dy = 0.00 \text{ \AA}$ (global energy minimum) and [R] $dy = 3.68 \text{ \AA}$ (global energy maximum).

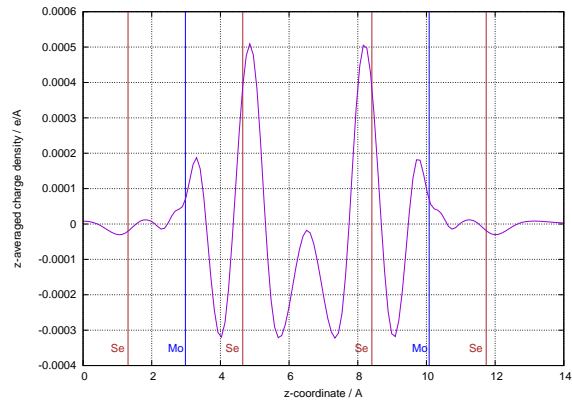
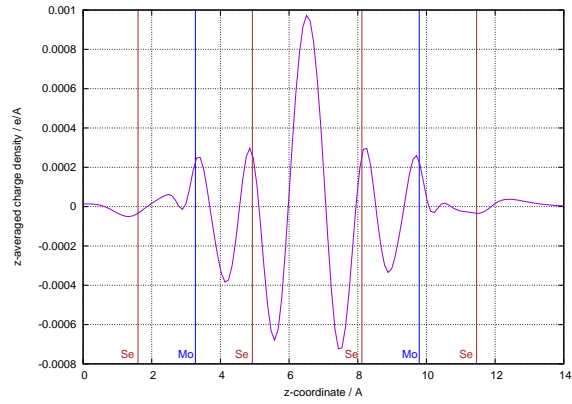


Figure 2: Plane-average charge density for the commensurate MoSe₂ bilayer at [L] $dy = 0.00 \text{ Å}$ (global energy minimum) and [R] $dy = 3.84 \text{ Å}$ (global energy maximum).

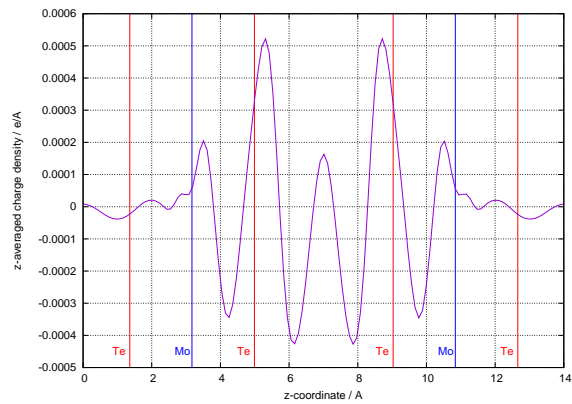
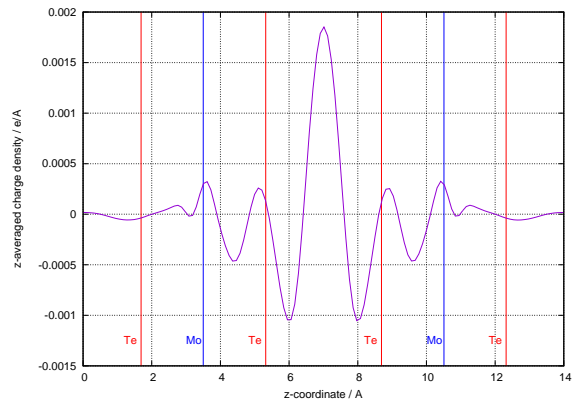


Figure 3: Plane-average charge density for the commensurate MoTe_2 bilayer at [L] $dy = 0.00 \text{ Å}$ (global energy minimum) and [R] $dy = 4.08 \text{ Å}$ (global energy maximum).

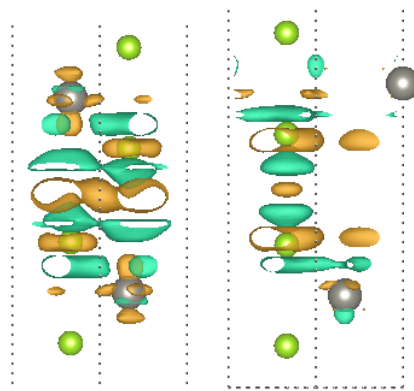


Figure 4: Charge density difference isosurfaces (isolevel $6.5 \times 10^{-5} \text{ e}/\text{\AA}^3$, positive = orange; negative = turquoise) for WSe₂ [L] at $dy = 0.00 \text{ \AA}$ (global energy minimum) and [R] $dy = 3.84 \text{ \AA}$ (global energy maximum)

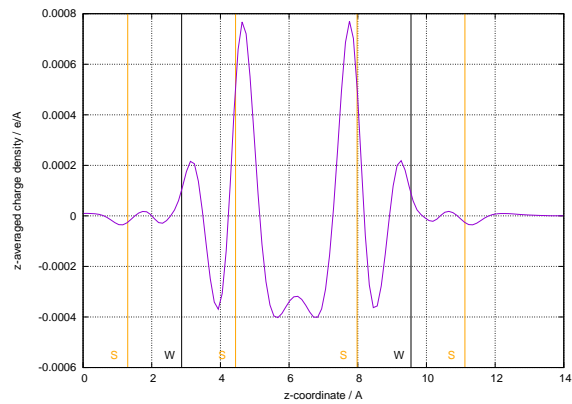
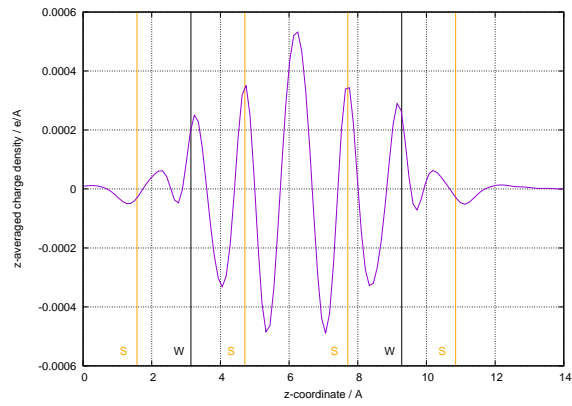


Figure 5: Plane-average charge density for the commensurate WS_2 bilayer at [L] $dy = 0.00 \text{ \AA}$ (global energy minimum) and [R] $dy = 3.68 \text{ \AA}$ (global energy maximum).

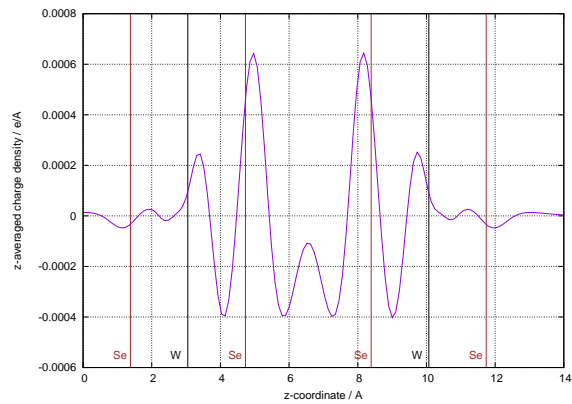
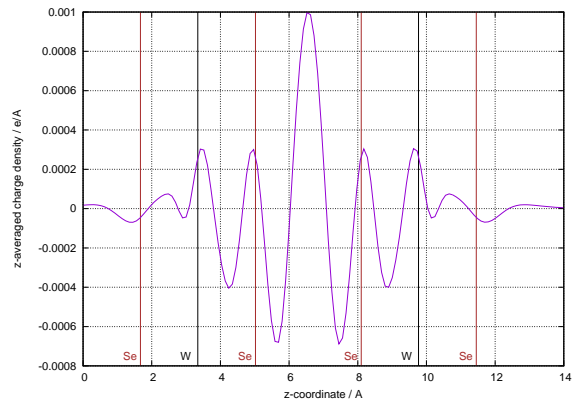


Figure 6: Plane-average charge density for the commensurate WSe_2 bilayer at [L] $dy = 0.00 \text{ Å}$ (global energy minimum) and [R] $dy = 3.84 \text{ Å}$ (global energy maximum).

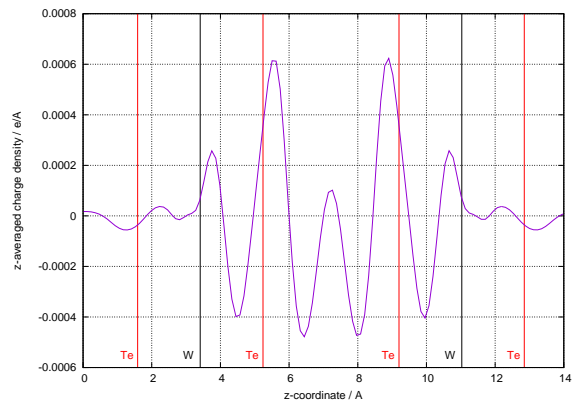
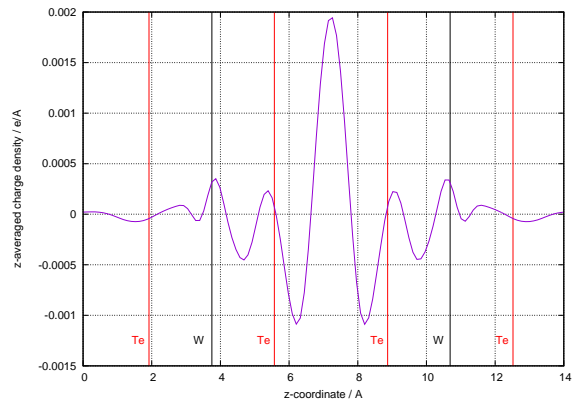


Figure 7: Plane-average charge density for the commensurate WTe_2 bilayer at [L] $dy = 0.00 \text{ \AA}$ (global energy minimum) and [R] $dy = 4.08 \text{ \AA}$ (global energy maximum).

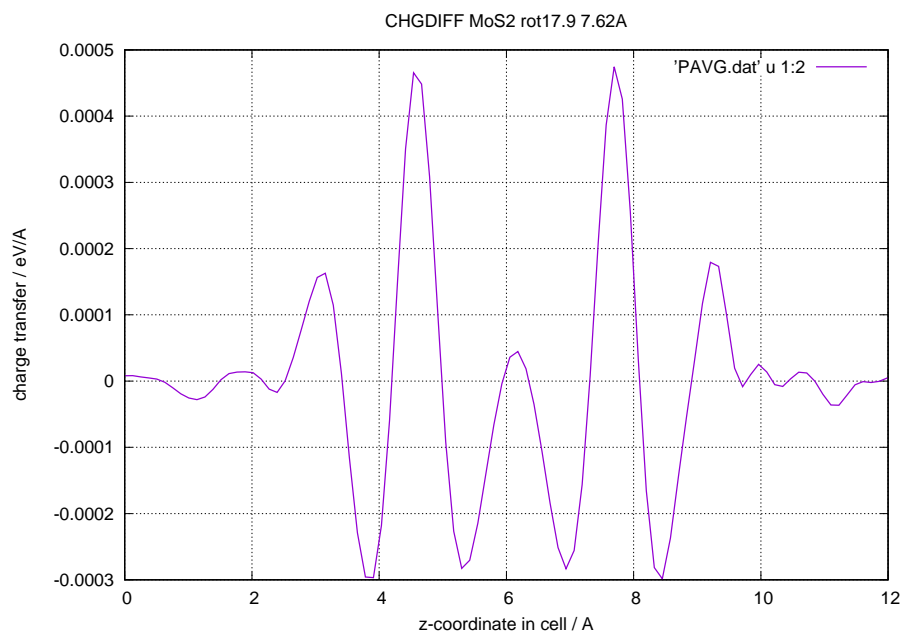


Figure 8: Planar averaged charge density for MoS₂ bilayer, mismatch angle 17.9 degrees, global energy minimum ($d_y = 7.62 \text{ \AA}$)

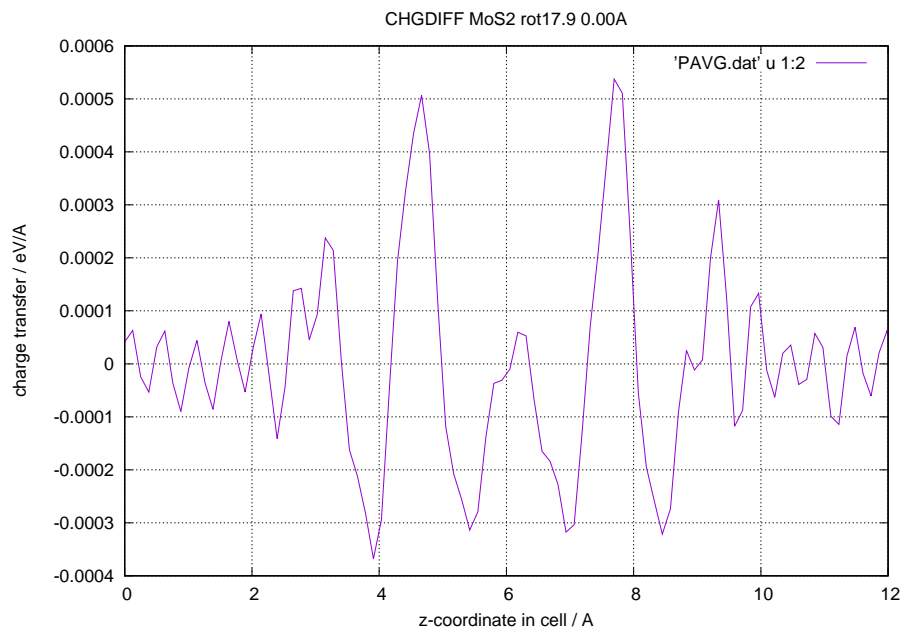


Figure 9: Planar averaged charge density for MoS₂ bilayer, mismatch angle 17.9 degrees, global energy maximum (dy = 0.00 Å)

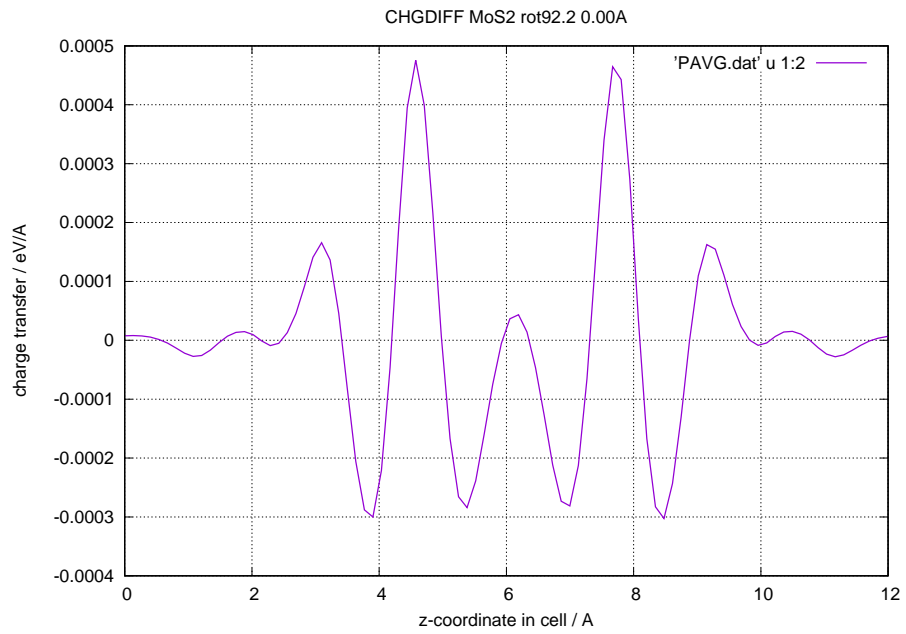


Figure 10: Planar averaged charge density for MoS₂ bilayer, mismatch angle 92.2 degrees, global energy minimum (dy = 0.00 Å)

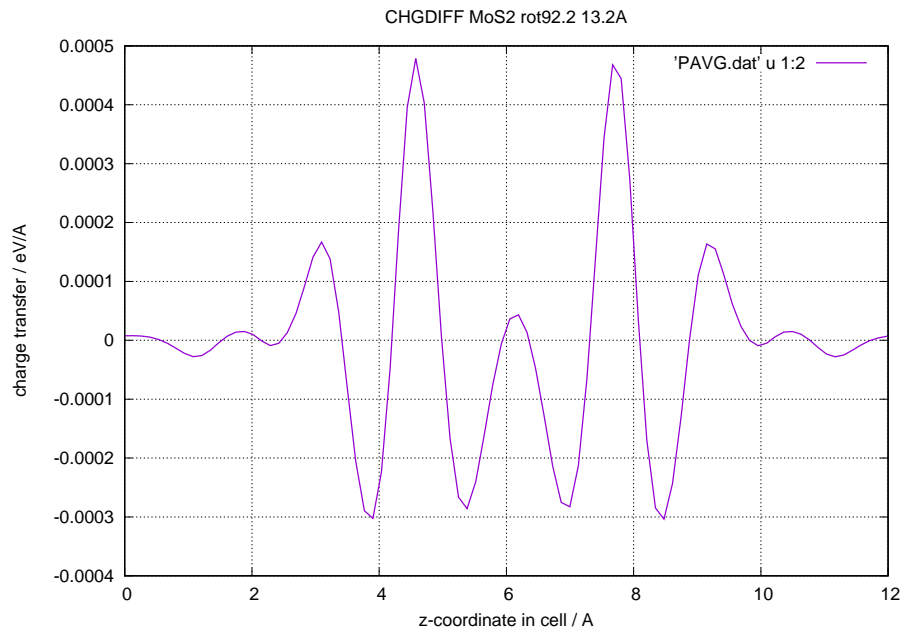


Figure 11: Planar averaged charge density for MoS₂ bilayer, mismatch angle 92.2 degrees, global energy maximum ($d_y = 13.20 \text{ \AA}$)

