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# The Chalcogen···Chalcogen Bonding in Molybdenum Disulfide, Molybdenum Diselenide and Molybdenum Ditelluride Dimers as Prototypes for a Basic Understanding of the Local Interfacial Chemical Bonding Environment in 2D Layered Transition Metal Dichalcogenides

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## Supplementary Information

**Table S1**: MP2(Full)/def2-TZVPPD computed uncorrected and BSSE corrected binding energies ($\Delta E$ and $\Delta E$(BSSE) in kcal mol$^{-1}$, respectively), and chalcogen···chalcogen ($r$(Ch···Ch)) bond distances of the nine dimers of Figure 2.

| Figure 3 | Dimer type | $\Delta E$ | $\Delta E$(BSSE) | $r$(Ch···Ch) /Å |
|---|---|---|---|---|
| a | ($MoTe_2$) ··· ($MoTe_2$) | -3.79 | -1.98 | 3.926 |
| b | ($MoSe_2$) ··· ($MoSe_2$) | -4.10 | -1.70 | 3.469 |
| c | (TeMoSe) ··· (SeMoTe) | -3.73 | -1.43 | 3.640 |
| d | (TeMoSe) ··· (TeMoSe) | -3.81 | -1.66 | 3.737 |
| e | ($MoTe_2$) ··· (SeMoTe) | -3.72 | -1.63 | 3.804 |
| f | ($MoTe_2$) ··· (TeMoS) | -3.64 | -1.88 | 3.958 |
| g | (SMoTe) ··· (SMoTe) | -3.37 | -1.90 | 3.640 |
| h | (SeMoS) ··· (SeMoS) | -3.48 | -1.87 | 3.431 |
| i | ($MoS_2$) ··· ($MoS_2$) | -3.09 | -2.02 | 3.331 |

**Table S2**: Some selected relaxed geometries of $MoCh_2$ (Ch = S, Se, Te) dimers, obtained with MP2(full) in conjunction with the def2-TZPPPD basis set
Redundant internal coordinates, Gaussian 16 format.

(a) $(MoTe_2)_2$ dimer
Mo,0,0.,4.1794504376,0.7873920888
Te,0,0.,1.9627937244,-0.0728906834
Te,0,0.,5.6572221132,-1.0726818861
Mo,0,0.,-4.1794504376,0.7873920888
Te,0,0.,-5.6572221132,-1.0726818861
Te,0,0.,-1.9627937244,-0.0728906834

(b) $(MoSe_2)_2$ dimer

Mo,0,0.,3.3826081972,0.7949308497
Se,0,0.,1.7345023727,-0.6691929337
Se,0,0.,5.1750552903,-0.4839183127
Mo,0,0.,-3.3826081972,0.7949308497
Se,0,0.,-5.1750552903,-0.4839183127
Se,0,0.,-1.7345023727,-0.6691929337

(c) (TeMoSe)…(SeMoTe)
Mo,0,0.,3.9585430441,0.7554494252
Se,0,0.,1.8201535301,0.2276992541
Te,0,0.,5.091745793,-1.3413288351
Mo,0,0.,-3.9585430441,0.7554494252
Te,0,0.,-5.091745793,-1.3413288351
Se,0,0.,-1.8201535301,0.2276992541

(d) (TeMoSe)…(TeMoSe)
Mo,0,0.,3.9583743367,0.7956286895
Se,0,0.,1.912958458,-0.022524056
Te,0,0.,5.3708019287,-1.1240568137
Mo,0,0.,-4.07596485,0.7537382472
Se,0,0.,-5.3288991508,-1.0542601321
Te,0,0.,-1.8372707226,-0.064886813

(e)$(MoTe_2)$…(SeMoTe)
Mo,0,0.,4.2139357568,0.7007840018
Te,0,0.,1.8452105746,0.4991779411
Te,0,0.,5.1077070445,-1.5011590543
Mo,0,0.,-4.1324219906,0.7046434037

Te,0,0.,-5.078572856,-1.4834922432
Se,0,0.,-1.9558585293,0.363685073

(f) ($MoTe_2$)…(TeMoS)
Mo,0,0.,4.2755324676,0.7340868573
Te,0,0.,1.9359802577,0.3098185779
Te,0,0.,5.3748651193,-1.3716433711
Mo,0,0.,-4.366639272,0.6528970719
S,0,0.,-5.1993585831,-1.2504085649
Te,0,0.,-2.0203799895,0.2088885509

(g)(SMoTe)…(SMoTe)
Mo,0,0.,3.8762298633,0.8174378551
Te,0,0.,1.7318253967,-0.2295985604
S,0,0.,5.1878583413,-0.7901111067
Mo,0,0.,-3.5115954071,0.7536730103
Te,0,0.,-5.3903073451,-0.7162881805
S,0,0.,-1.8940108491,-0.5514738959

(h) (SeMoS)…(SeMoS)
Mo,0,0.,3.477171836,0.8112124656
Se,0,0.,1.6632878298,-0.4414101703
S,0,0.,4.9802704211,-0.6184061347
Mo,0,0.,-3.2814961034,0.7397195814
Se,0,0.,-5.0790693643,-0.5317925784
S,0,0.,-1.7601646192,-0.6756840415

(i) $(MoS_2)_2$ dimer
Mo,0,0.,3.1765115035,0.7589013567
S,0,0.,1.6652551526,-0.6630494987
S,0,0.,4.8560758724,-0.4540322803
Mo,0,0.,-3.1765115035,0.7589013567
S,0,0.,-4.8560758724,-0.4540322803
S,0,0.,-1.6652551526,-0.6630494987

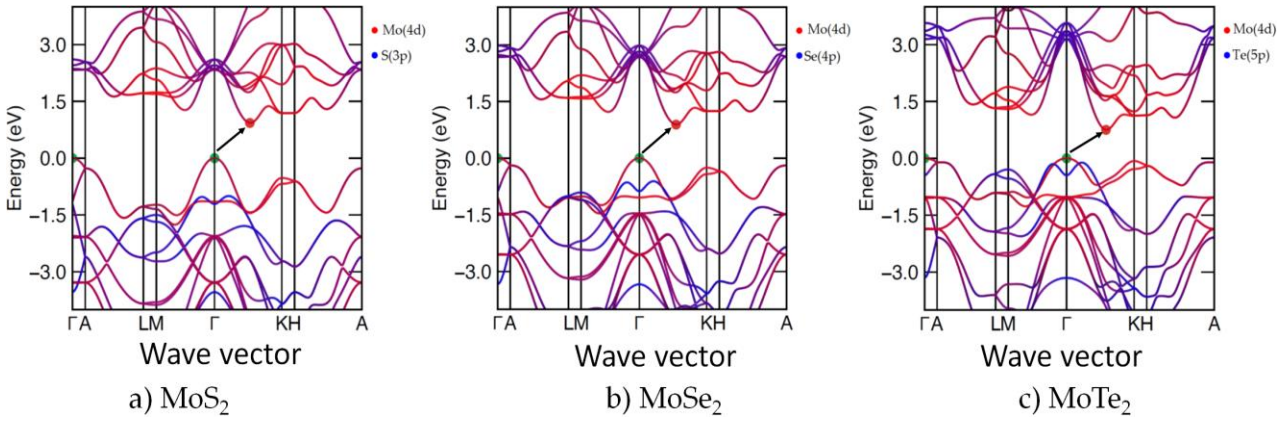


**Figure S1**. The atom/orbital-projected band structures of all the three bulk systems $MoCh_2$ (Ch = S, Te, Se), obtained using SCAN-*rVV10*. The VBM and CBM are found at Γ and between K-Γ, respectively.