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Structural and electronic behaviour of MoS2, MoSe2 and MoTe2 at high pressure

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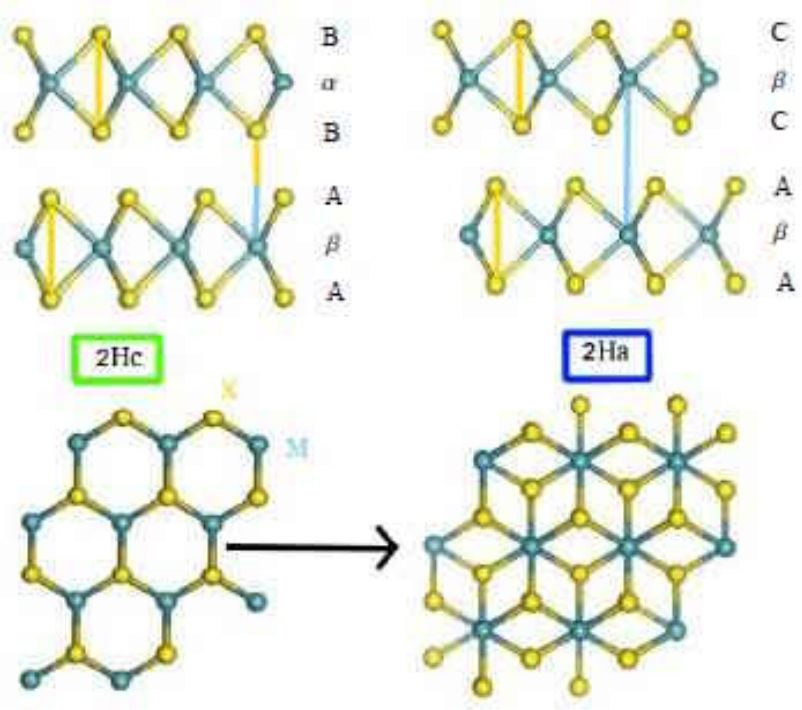
Using ab initio calculations and metadynamics simulations we studied the behaviour of layered semiconducting transition metal dichalcogenides, MoX2 (X = S, Se, Te) at high pressure with focus on structural transitions and metallization [1,2]. We found that concerning structure, the behaviour of MoS2 is different from that of MoSe2 and MoTe2. In MoS2 pressure induces at 20 GPa a structural transition where layer sliding takes place, bringing the initial 2Hc stacking to a 2Ha stacking typical of e.g. 2H-NbSe2. This finding naturally explains previous X-ray diffraction and Raman spectroscopy data and was very recently confirmed by new X-ray diffraction experiments[3]. On the other hand, this transition does not occur in MoSe2 and MoTe2 where instead the initial 2Hc stacking remains stable. Besides structural changes pressure in MoS2 induces also a semiconductor - semimetal transition which takes place by band overlap and closing of indirect band gap. This electronic transition occurs in the same region where the structural transition takes place, at 25 GPa in the 2Hc phase and at 20 GPa in the 2Ha phase. In case of MoSe2 and MoTe2 a very similar electronic transition leading to semimetal is predicted to occur at 28 GPa and 13 GPa, respectively. All three materials exhibit after metallization a low density of states at the Fermi level implying low superconducting temperature (if any). Due to absence of structural transition in the metallization region MoSe2 and MoTe2 could be suitable candidate materials for observation of the excitonic insulator phase.

[1] *Liliana Hromadova, Roman Martonak and Erio Tosatti, Phys. Rev. B, 2013, 87, 144105,* ***[2]*** *Michaela Riflikova, Roman Martonak and Erio Tosatti, submitted,* ***[3]*** *Nirup Bandaru et al., J. Phys. Chem. C, 2014, DOI: 10.1021/jp410167k*



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