LIVRO DE RESUMOS

SIFSC

DÉCIMA SEMANA INTEGRADA DA GRADUAÇÃO E PÓS-GRADUAÇÃO DO INSTITUTO DE FÍSICA DE SÃO CARLOS - USP

2020

Universidade de São Paulo
Instituto de Física de São Carlos

X Semana Integrada do Instituto de Física de São Carlos

Livro de Resumos

São Carlos
2020

Semana Integrada do Instituto de Física de São Carlos

SIFSC 10

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Ficha catalográfica elaborada pelo Serviço de Informação do IFSC

Semana Integrada do Instituto de Física de São Carlos
(10: 03-05 nov.: 2020: São Carlos, SP.)
Livro de resumos da X Semana Integrada do Instituto de Física de São Carlos/ Organizado por Joao H. Melo Inagaki [et al.]. São Carlos: IFSC, 2020.
321p.
Texto em português.
1.Física. I. Inagaki, Joao H. de Melo, org. II.Titulo.

ISBN: 978-65-993449-0-9 CDD 530

PG155

Band gaps beyond Anderson rule and imbalance of interlayer charge carrier transfer in van der Waals heterostructures of transition metal dichalcogenides

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With the expanding knowledge of two-dimensional materials, the fabrication of van der Waals (vdW) heterostructures through the vertical stacking of different monolayer materials (1) has been proposed as a platform to design materials for several applications, such as photovoltaics and electrocatalysis. (2) However, despite being dominated by weak vdW interactions, interlayer coupling can play an important role in the properties of the vdW heterostructures, and the understanding of this aspect still needs to be improved. In particular, key parameters to design semiconductor heterojunctions are the band alignments and resulting band gaps, and also the mechanisms of interlayer charge transfer that occur after electron excitations in these systems. To shed light into these questions we performed a density functional theory (DFT) investigation of vdW heterobilayers formed of 6 transition metal dichalcogendies monolayers (MQ_2 ; M = Mo, Ni, Pt; Q = S, Se). (3) We employed the Vienna Ab Initio Simulation Package (VASP) to calculate the electronic band structures, and the interlayer charge transfer was studied with the Time-dependent DFT formalism combined with molecular dynamics, as implemented in the Spanish Initiative for Electronic Simulations with Thousands of Atoms (SIESTA) code. We found that for 8 heterobilayers the band gaps can be obtained through the Anderson Rule within a 0.10 eV accuracy, whereas the remaining systems have their band gaps increased or decreased by up to 0.28 eV from Anderson rule values, and we identified two important mechanisms that cause these variations. In one, interfacial hybridizations of electronic states in the valence band create electronic states with higher energy than the original top valence band of isolated monolayers, thus leading to a decrease in the band gap. This effect is more pronounced in junctions that have Ni or Pt in both layers, in which a large number of bands are involved in the interactions, whereas in junctions that contain Mo the effect can be traced mainly to the interactions between Mo-d_{z^2} + Q-p_z states in MoQ_2 and Q-p_z states in (Ni,Pt)Q_2. The other effect is responsible for increasing the band gap, and occurs in heterojunctions with type-II band alignment, for which an electric dipole due to the formation of the interface leads to a relative shift of band energies between the two layers. The monolayer band offsets of the $MoS_2/PtSe_2$ heterojunction suggest the formation of a type-I junction, with both valence band maximum (VBM) and conduction band minimum (CBM) located at $PtSe_2$, but upon the formation of the heterobilayer, a shared VBM state is created. A photoexcitation involving the VBM and CBM of MoS_2 is expected to cause holes and electrons to transfer to lower energy states in $PtSe_2$. Our results show that electron transfer occurs at a faster rate than hole transfer, which is explained by the stronger coupling of conduction band states compared to valence band, due to a smaller energy difference. Furthermore, electron transfer is secondarily enhanced by a level crossing induced by the interfacial dipole that originates from the imbalance in charge carriers transfer.

Referências:

1 GEIM, A. K.; GRIGORIEVA, I. V. Van der Waals heterostructures. **Nature** , v. 499, n. 7459, p. 419-425 , 2013. 2 LI, C. Engineering graphene and TMDs based van der Waals heterostructures for photovoltaic and photoelectrochemical solar energy conversion. **Chemical Society Reviews** , v. 47,

n. 13, p. 4981-5037, 2018. 3 BESSE, R.; LIMA, M. P.; DA SILVA, J. L. F. First-principles exploration of two-dimensional transition metal dichalcogenides based on Fe, Co, Ni, and Cu groups and their van der Waals heterostructures. **ACS Applied Energy Materials** , v. 2, n. 12, p. 8491-8501, 2019.