Abstract Submitted
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First-Principles Studies of Heterostructures with Transition Metal Dichalcogenides.[1] XIN-JUN WANG, University at Buffalo, PREDRAG LAZIC, Institute Rudjer Boskovic, ALEX MATOS-ABIAGUE, IGOR ZUTIC, University at Buffalo — We use first-principles calculations to study electronic properties of van der Waals (vdW) heterostructures with transition metal dichalcogenides (TMDs). Using a novel CellMatch procedure for optimizing the strain in vdW heterostructures [1], unit cells of a TMD and another material are combined in a relaxed common supercell of their vdW heterostructure. Our results are examined in TMD heterostructures with graphene and topological insulators, representing materials with a weak and strong spin-orbit coupling, respectively. We explore the possibility for tunable proximity effects [2,3] which may not be apparent from the individual vdW materials. \[1] P. Lazic, Comp. Phys. Commun. 197, 324 (2015). \[2] R. V. Gorbachev, J. C. W. Song, G. L. Yu, A. V. Kretinin, Y. F. Withers, A. M. Cao,. V. Grigorieva, K. S. Novoselov, L. S. Levitov, and A. K. Geim, Science 346, 448 (2014).\[3] P. Lazic, K. D. Belashchenko, and I. Zutic, Phys. Rev. B 93, 241401(R) (2016).

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Igor Zutic
University at Buffalo

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