Brazil's Sociedade Brasileira de Fisica membership pending

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Band Offsets Engineering for van der Waals Heterostructure Devices DANIEL S. KODA, Instituto Tecnológico de Aeronáutica, 12228-461 São José dos Campos, Brazil, FRIEDHELM BECHSTEDT, Friedrich-Schiller-Universität, Max-Wien-Platz 1, D-07743 Jena, Germany, MARCELO MARQUES, LARA K. TELES, Instituto Tecnológico de Aeronáutica, 12228-461 São José dos Campos, Brazil — Two-dimensional crystals (2D) and their stacks in van der Waals heterostructures became prospective for novel devices and physics. To surmount commensurability limitations within first-principles investigations, the coincidence lattice method is developed[1], enabling studies on interlayer twist[2] and quasiparticle corrections despite limited computational resources. Interesting properties are observed within stacked systems, such as structural deformation on contact, strong orbital hybridization, and tunable band offsets by application of pressure and vertical electric fields[3]. These studies could help to develop versatile electronic and optoelectronic devices and unravel new physics within 2D interfaces.

[1]D. S. Koda, F. Bechstedt, M. Marques, and L. K. Teles, *J. Phys. Chem. C* **120** (2016) 10895.
[2]D. S. Koda, F. Bechstedt, M. Marques, and L. K. Teles, *J. Electron. Mater.* (2016).
[3]D. S. Koda, F. Bechstedt, M. Marques, and L. K. Teles, submitted to the *J. Phys. Chem. Lett.* (2016).

Daniel S. Koda
Instituto Tecnológico de Aeronáutica, 12228-461 São José dos Campos, Brazil

Date submitted: 17 Nov 2016 Electronic form version 1.4