Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Stacking van der Waals materials[1] PREDRAG LAZIC, Rudjer Boskovic Institute — We have developed a code (CellMatch [1]) that searches for common unit cells of two layered structures. Typically the two structures will not have a common lattice constant so a compromise is needed between the size of the cell and the strain imposed on one of the structures. Whether it is a heterostructure of two van der Waals materials or a vdW material on a substrate CellMatch searches through possible common unit cells yielding a strain for each result. We demonstrate the use of the code in combination with Density Functional Theory calculations - by studying cases of MoS2 growth on the sapphire surface, and hBN on the Ir(111). [1] P. Lazic, Comput. Phys. Comm. **197**, 324 (2015).

[1]P. L. was supported by the Unity Through Knowledge Fund, Contract No. 22/15 and H2020 CSA Twinning Project No. 692194, RBI-T-WINNING.

Predrag Lazic
Rugjer Boskovic Inst

Date submitted: 09 Nov 2016 Electronic form version 1.4