

Materials List for:

## Probe Type II Band Alignment in One-Dimensional Van Der Waals Heterostructures Using First-Principles Calculations

HuiHui Hu<sup>1</sup>, DeBen Lu<sup>1</sup>, Kun Peng Dou<sup>1</sup>, Xing-Qiang Shi<sup>2</sup>

<sup>1</sup>College of Information Science and Engineering, Ocean University of China

<sup>2</sup>Department of Physics, Southern University of Science and Technology

Correspondence to: Kun Peng Dou at [doukunpeng@ouc.edu.cn](mailto:doukunpeng@ouc.edu.cn)

URL: <https://www.jove.com/video/60180>

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### Materials

Name	Company	Catalog Number	Comments
Nanotube Modeler	Developed by Dr. Steffen Weber	NanotubeModeler1.8	<a href="http://www.jcrystal.com/products/wincnt/NanotubeModeler.exe">http://www.jcrystal.com/products/wincnt/NanotubeModeler.exe</a>
P4VASP	Orest Dubay	p4vasp 0.3.30	Open source, available at <a href="http://www.p4vasp.at">www.p4vasp.at</a>
v2xsf	Developed by Dr. Jens Kunstmann	v2xsf	<a href="http://theory.chm.tu-dresden.de/~jk/software.html">http://theory.chm.tu-dresden.de/~jk/software.html</a>
VASP software	Computational Materials Physics, Dept. of Physics, University of Vienna	vasp.5.4.1	<a href="https://www.vasp.at">https://www.vasp.at</a>
VMD software	Theoretical and Computational Biophysics Group, University of Illinois at Urbana-Champaign	vmd1.9.3	<a href="https://www.ks.uiuc.edu/Research/vmd">https://www.ks.uiuc.edu/Research/vmd</a>
xcrysden	Dept. of Physical and Organic Chemistry, Jozef Stefan Institute	XCrySDen1.5.60	<a href="http://www.xcrysden.org/">http://www.xcrysden.org/</a>
Xmakemol	Developed by M. P. Hodges	xmakemol5.16	<a href="https://www.nongnu.org/xmakemol/XmakemolDownloads.html">https://www.nongnu.org/xmakemol/XmakemolDownloads.html</a>
Xmgrace software	Grace Development Team under the coordination of Evgeny Stambulchik	xmgrace5.1.25	<a href="http://plasma-gate.weizmann.ac.il/Grace/">http://plasma-gate.weizmann.ac.il/Grace/</a>