2021 HybriD^3 Theory Training Workshop

Lectures :

Prof. Elena Jakubikova (NCSU)
Prof. Weitao Yang (Duke)
Prof. Noa Marom (Carnegie Mellon)

Tutorial :

Dr. Yi Yao (UNC/Duke)
Ms. Sampreeti Bhattacharya (UNC)
Ms. Xixi Qin (Duke)
Mr. Ruyi Song (Duke)

Organizers : Prof. Volker Blum (Duke) & Prof. Yosuke Kanai (UNC)

We gratefully acknowledge support of the **HybriD^3 project** by the National Science Foundation under Awards Number 1728921, 1729297, and 1729383.

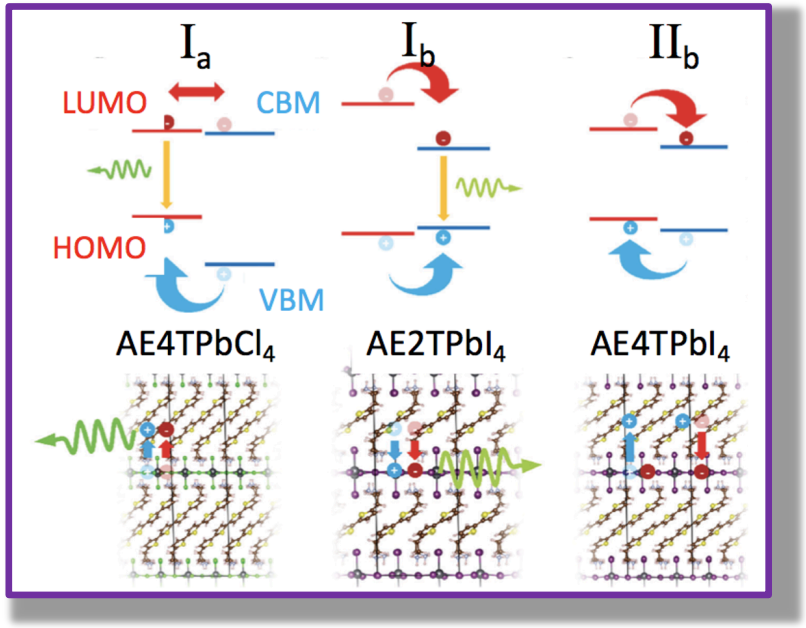
Duke UNIVERSITY NC STATE UNIVERSITY THE UNIVERSITY of NORTH CAROLINA at CHAPEL HILL NSF

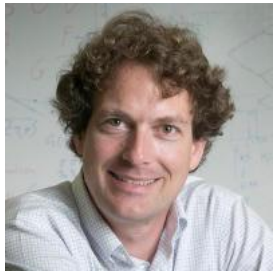
What Is HybriD^3 ?

Design, Discovery and Dissemination (D^3) of new hybrid organic-inorganic semiconductors

NSF Program : Materials Genome Initiative

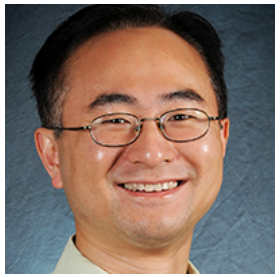
Designing Materials to Revolutionize and Engineer our Future (DMREF)





Volker Blum
Duke
Theory/Comp.

David Mitzi
Duke
Materials



Wei You
UNC-CH
Synthesis

Yosuke Kanai
UNC-CH
Theory/Comp.

Kenan Gundogdu
NCSU
Spectroscopy

Franky So
NCSU
Device

http://hybrid3.duke.edu/

HybriD^3

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Welcome

Hybrid organic-inorganic materials offer a unique opportunity for the discovery and refinement of new functional semiconductor materials with fine-tuned properties, controlled at the atomic scale by organic chemistry and organic-inorganic synthesis and processing. The HybriD^3 project accelerates the *Design, Discovery and Dissemination* (D^3) of new crystalline organic-inorganic hybrid semiconductors in a collaborative effort between six teams of researchers located at three major universities in the Research Triangle: Duke University, University of North Carolina Chapel Hill and North Carolina State University.

The team will concentrate their effort on identifying new organic-inorganic hybrid perovskites, aiming, for

RECENT NEWS

Publication Mentioned on Perovskite-Info Website!

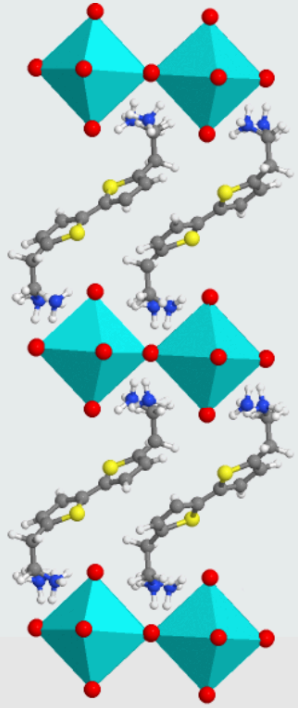
DECEMBER 21, 2020

Congratulations to Akash Singh, Manoj K. Jana, and David B. Mitzi.

https://materials.hybrid3.duke.edu/

HybriD³ database | Home | Search | HybriD³ project | Contributors | Software behind the database | Contact | Login | Register

Welcome to the HybriD³ materials database

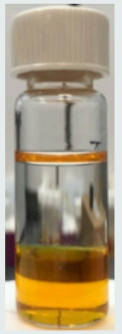


The HybriD³ materials database provides a comprehensive collection of experimental and computational materials data for crystalline organic-inorganic compounds, predominantly based on the perovskite paradigm.

The data is available under the Creative Commons license with attribution clause, described here and, in its full text, here. We also intend to offer the data for inclusion in broader materials databases in order to maximize its accessibility.

Please contact us if you wish to add specific materials to the database - the database is intended to be accessible by the community and we would be delighted to hear from you.

Learn more | Start searching



PROGRAM SCHEDULE

Day 1: January 19 (Tuesday)

9:10 - 9:55 am : "DFT for (almost) beginners", **Prof. Elena Jakubikova (NCSU)**

10:00 -10:45 am : "Exchange-Correlation Functionals in DFT", **Prof. Weitao Yang (Duke)**

11:00 -11:45 am : "Accurate Materials Predictions with DFT and Machine Learning", **Prof. Noa Marom (Carnegie Mellon Univ.)**

Day 2: January 20 (Wednesday)

9:00 - 9:45 am : "Nuts-and-Bolts of DFT", **Prof. Volker Blum (Duke)**

10:00 am - 1:00 pm : Hands-on tutorial session: Properties of Molecules and Solids

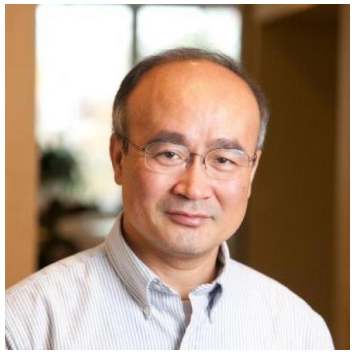
Day 3: January 21 (Thursday)

9:00 - 9:45 am : "First-Principles Molecular Dynamics with DFT", **Prof. Yosuke Kanai (UNC)**

10:00 am - 1:00 pm : Hands-on tutorial session: Molecular Dynamics

Tutorials will be based on the FHI-aims code. The task will be focused on science, not code-specific objectives.

Elena Jakubikova
NCSU



Weitao Yang
Duke

Noa Marom
Carnegie Mellon