# New Materials from Simulations

**Julian Gebhardt**

*Max Planck Institute for the Structure and Dynamics of Matter Luruper Chaussee 149 22761 Hamburg, Germany*
*E-mail: julian.gebhardt@mpsd.mpg.de*

Electronic-structure theory has become a powerful tool to design and analyze new materials with target properties. I will give an overview of our work from the design stage towards fabrication, focusing on the aspects of theoretical guidance. In particular, I will report on the bottom-up synthesis of organic two-dimensional networks via substrate assisted covalent bond formation after controlled self organization[1, 2] as well as structural perovskite modifications targeted to overcome stability problems of next generation perovskite photovoltaics.[3–6]

## References

[1] C. Steiner, J. Gebhardt, M. Ammon, Z. Yang, A. Heidenreich, N. Hammer, A. Görling, M. Kivala, S. Maier, *Nat. Commun.* **2017**, *8*, 14765.

[2] Z. Yang, J. Gebhardt, T. A. Schaub, T. Sander, J. Schönamsgruber, H. Soni, A. Görling, M. Kivala, S. Maier, *Nanoscale* **2018**, *10*, 3769–3776.

[3] J. Gebhardt, A. M. Rappe, *Adv. Mater.* **2018**, *Accepted*, 1802697.

[4] J. Gebhardt, A. M. Rappe, *ACS Energy Lett.* **2017**, *2*, 2681–2685.

[5] J. Gebhardt, A. M. Rappe, *J. Mater. Chem. A* **2018**, *6*, 14560.

[6] J. Gebhardt, Y. Kim, A. M. Rappe, *J. Phys. Chem. C* **2017**, *121*, 6569–6574.