Keeping Supercomputers Busy: Configuration Space Exploration and *GW* Calculations

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In this talk I will share my users perspective on running resource-intensive calculations with FHI-aims within my work on materials for organic and dye-sensitized solar cells. In order to make meaningful predictions for such systems, it is important to obtain an accurate description of the structure and electronic properties of the materials and interfaces involved. Structure prediction may require configuration space exploration, which is typically time-consuming, owing to the need to sample several hundred trial structures. The proper description of fundamental gaps and level alignment at interfaces requires memory-intensive *GW* calculations. I will discuss some examples of metal-organic dyes [1], TiO_2 clusters [2], dye-sensitized TiO_2 clusters [3], and polycyclic aromatic hydrocarbons (PAHs) [4], in terms of the required computational effort and the results obtained.

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[2] N. Marom, M. Kim, and J. R. Chelikowsky, Phys. Rev. Lett. 108, 106801 (2012).
[3] N. Marom, J. E. Moussa, X. Ren, A. Tkatchenko, and J. R. Chelikowsky, Phys. Rev. B 84, 245115 (2011).
[4] J. E. Moussa, N. Marom, and J. R. Chelikowsky, to be published.