Deep Learning for Molecular OF-DFT

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Density Functional Theory (DFT), arguably the most widely used methodology for the study of the electronic properties of materials, is commonly described using the Kohn-Sham (KS) formalism. However, due to its unfavorable computational cost scaling, it is often limited to systems with a few hundred atoms at maximum. In this project, we employ AI models to directly obtain the electron density given only the external potential felt by the electrons in molecular systems. Thus, just knowing the external potential is sufficient to completely solve the DFT problem, avoiding any need for self-consistent calculations. A ley insight of this work is that these functions can be considered as different representations of the same molecule (Figure 1), and as such, we can use image transformation techniques [1] to learn their mapping. This work opens the possibility of the application of DFT to much larger systems, with orders of magnitude decrease in computational cost.

References

[1] Phillip Isola, Jun-Yan Zhu, Tinghui Zhou and Alexei A. Efros, arXiv, 1611.07004 (2016).

Figures

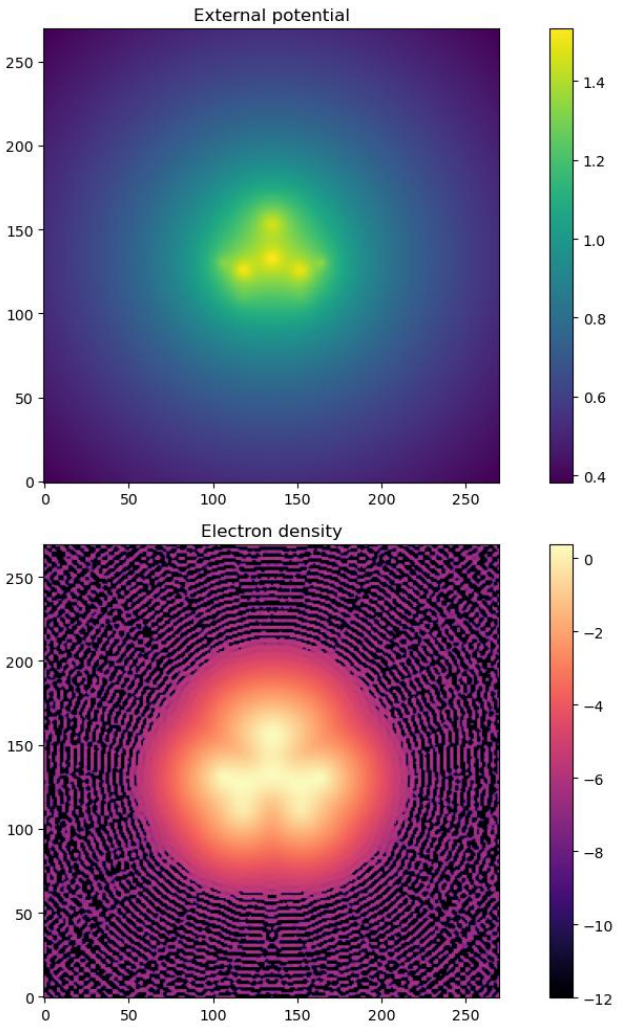

Figure 1. (a) External potential logarithmic map in arbitrary units of a molecule, 2D slice of a 3D tensor. (b) Analogous map for electron density. We can appreciate how the two images represent the same molecule in different ways, and how the structure of the molecule is visible in both.