Learning workflow-aware materials representations - from electron densities to tomographic fusion

Tejs Vegge[1,2,†]

[1]Pioneer Center for Accelerating P2X Materials Discovery, CAPeX

[2]Technical University of Denmark, DTU Energy, 2800 Kgs. Lyngby, Denmark

† corresponding author's email: teve@dtu.dk

Machine learning for materials is increasingly judged not only by predictive accuracy, but whether it accelerates end-to-end discovery workflows, e.g., from electronic-structure calculations and high-throughput screening to self-driving laboratories [1]. A particularly powerful representation for this purpose is the electron density, which is physically grounded, transferable across tasks, and can serve as a universal intermediate for downstream observables. Yet practical impact depends on representational efficiency [2].

We discuss two complementary density representations designed explicitly for workflow impact. In molecules, ELECTRA [3] reconstructs charge densities using compact mixtures of anisotropic Gaussians ("floating orbitals"). A key obstacle for equivariant learning is that strict symmetry constraints can lock outputs to input symmetries, which is overcome using a rotation-equivariant symmetry-breaking mechanism that enables expressive orbital placement while preserving the correct transformation behavior of the density.

For periodic materials, ELECTRAFI [4] extends the Gaussian ansatz but delegates global periodicity to the analytic structure and enabling direct reconstruction of the full periodic density through a single inverse FFT. This removes expensive real-space grid probing and periodic image summation, yielding sub-second inference and >100x speedups over strong grid-based baselines while maintaining state-of-the-art accuracy. When used to initialize self-consistent DFT, ELECTRAFI reduces total DFT compute cost significantly.

Finally, we connect density-based representations to a tomographic perspective on materials descriptors: properties and representations can be viewed as complementary projections of an underlying material object. Fusing multiple, task-relevant descriptors can progressively reduce uncertainty, suggesting a principled route to multimodal, workflow-aware representations that remain physically grounded yet operationally useful in closed-loop discovery [5,6].

References:

[1] Back et al., Accelerated chemical science with AI, Digital Discovery (2024).
[2] Canty et al., Science acceleration with self-driving laboratories, Nat. Commun. (2025).
[3] Elsborg et al., ELECTRA: A Cartesian Network for 3D Charge Density Prediction with Floating Orbitals, NeurIPS Spotlight (2025).
[4] Elsborg et al., ELECTRAFI: periodic charge densities from local Gaussians, arXiv:2601.19966 (2026).
[5] Ortega-Ochoa et al., Tomographic interpretation of materials representations, arXiv:2501.18163 (2025).
[6] Ortega-Ochoa et al., Deep tomography for molecular and materials representations, Digital Discovery (2026).