GLASS: A Geometric Local Attention-Based Model to Design Superconducting Structures

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Superconductors, materials that achieve zero resistivity when cooled below their critical temperature, show promising applications in quantum computing, nuclear fusion, and electrical transmission. However, the development of superconductors currently relies on a slow and expensive trial-and-error process. To rapidly accelerate the discovery of new superconductors, this research proposes GLASS, a novel, deep-learning approach to generate high-temperature superconductors. GLASS is the first-ever end-to-end pipeline to utilize a molecule’s 3D crystal structure for superconductor design. GLASS consists of two parts: a novel Conditional Deep-Feature-Consistent Variational Autoencoder (Cond-DFC-VAE) that generates new potential superconductors, and a novel Geometric-Information-Enhanced Crystal Graph Neural Network (GeoCGNN) that models electron-phonon interactions to predict a material’s critical temperature. GLASS designs superconductors efficiently and effectively. GLASS's generative approach allows it to freely explore the entirety of crystal space, while its high physical fidelity, with 87% of GLASS-designed superconductors containing an Ef < 0, ensures that these molecules are stable and synthesizable. Generating 10,000 new superconductors, GLASS discovered 7 new high-temperature superconductors with a critical temperature over 100K. The validity of these results is reinforced by GLASS's critical temperature prediction accuracy, which outperformed all state-of-the-art methods by over 50%. Not only does GLASS design targeted, high-temperature superconductors, but it does so 1,400,000x faster than the traditional trial-and-error process. Through the creation of a novel pipeline for superconductor discovery, GLASS pushes us closer to a quantum, carbon-free future.

Awards Won:

Third Award of $1,000