CarbNN: A Novel Active Transfer Learning Neural Network to Build De Novo Metal Organic Frameworks (MOFs) for Carbon Capture

Redkar, Neel (School: Dougherty Valley High School)

Over the past decade, climate change has become an increasing problem with one of the major contributing factors being carbon dioxide (CO_2) emission—almost 51% of total US carbon emissions are from factories. The effort to prevent CO_2 from going into the environment is called carbon capture. Carbon capture decreases CO_2 and also yields steam that can be used to produce energy, decreasing net energy costs by 25-40%, though the isolated CO_2 must be sequestered through expensive means. Current materials used in CO_2 capture are lacking either in efficiency, sustainability, or cost. Electrocatalysis of CO_2 is a new approach where CO_2 can be split and the components used industrially as fuel, saving transportation costs, creating financial incentives. Metal Organic Frameworks (MOFs) are crystals made of organo-metals that can adsorb, filter, and electrocatalyze CO_2. The current available MOFs for capture & electrocatalysis are expensive to manufacture and inefficient. Thus, the engineering goal for this project was to design a novel MOF that can adsorb CO_2 and use electrocatalysis to convert it to CO and O efficiently while maintaining a low manufacturing cost. A novel active transfer learning neural network was developed, utilizing transfer learning due to limited available data on 15 MOFs. Using the CSD with 10K MOFs, the model used incremental mutations to fit a trained fitness hyper-heuristic function. Eventually, a Se-MOF ($C_{18}MgO_{25}Se_{11}Sn_{20}Zn_5$) was converged on. Through analysis of predictions & the literature base, it was shown to be more effective & less costly than existing MOFs, showing the model had a complex understanding of the material space. This novel network could be implemented for other gas separations and catalysis applications using sparse datasets.

Awards Won:

Second Award of $2,000

Fondazione Bruno Kessler: Award to participate in summer school "Web Valley"

Association for the Advancement of Artificial Intelligence: AAAI Memberships for 1st, 2nd, and 3rd Prize Winners (in-kind award / part of the 1st-3rd prize)

Association for the Advancement of Artificial Intelligence: AAAI Membership for the School Libraries of All 8 Winners (in-kind award / part of 1st-3rd prize and honorable mentions' prize)

Association for the Advancement of Artificial Intelligence: Second Award of $1,000