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Chemical Material Research using Machine Learning Platform

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I would like to introduce two web-based ML platforms, SimPL-ML and ChemAI, that enable the user to build an ML prediction model through a simple process using their own data. SimPL-ML provides a platform environment where anyone can efficiently perform ML tasks regardless of field.[1] Meanwhile, ChemAI can predict structure-based (graph-based) properties using material structure information such as cif or SMILES and provides various types of toolkits implemented by advanced deep learning models. ChemAI also contains a unified architecture of neural networks (DopNet) that accurately predicts the material's properties of the doped inorganic materials. All ML tasks in two ML platforms are conducted under an easily accessible web-based environment. A user interface environment has been built to use even researchers with little experience in code development freely. Our ML platforms are expected to help more researchers in materials chemistry enable advanced materials research through ML.

[1] **Seunghun Jang***, Gyoung S Na, Jungho Lee, Jung Ho Shin, Hyun Woo Kim, Hyunju Chang*, "An Easy, Simple, and Accessible Web-based Machine Learning Platform, SimPL-ML", *Integrating Materials and Manufacturing Innovation* **2022**, 11, 85-94