



Showcasing research from Professor Back's laboratory,
Department of Chemical and Biomolecular Engineering,
Sogang University, Seoul 04107, Republic of Korea.

A chemically inspired convolutional neural network using
electronic structure representation

The machine learning model uses the initial density of
states to predict the stability of materials, bypassing
geometry optimization. Therefore, the model can quickly
discover stable materials in a large chemical space with low
computational cost.

As featured in:



See Jonggeol Na, Seoin Back *et al.*,
J. Mater. Chem. A, 2023, **11**, 10184.