Theoretical Investigation of Hydrogen Desorption Process in Hydrogen Boride sheet for Catalytic Application

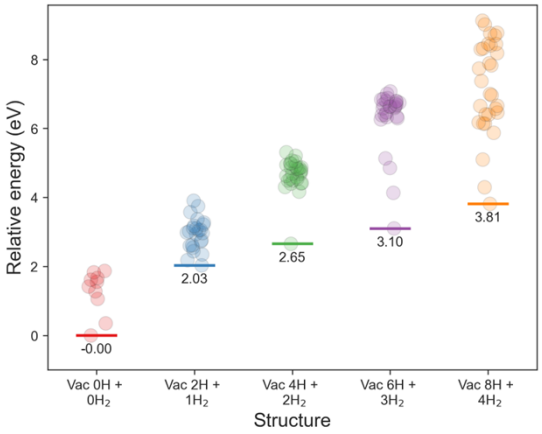
Osaka university, Department of Precision Science and Technology, Kurt Irvin M. Rojas

Purpose Explore the effect of hydrogen desorption in hydrogen boride (HB) sheet structure

Outline
(1) Global optimization of H-vacant HB using machine-learning,
(2) structure filtering and clustering,
(3) comparative analysis

Result
(a) New structures arising from the structure search was observed
(b) Stability of the first desorption differs by 2 eV
(c) Succeeding desorption have lower stability but has less difference

Computing system:	SQUID General Purpose CPU nodes
node-hour	13,410 node-hour
memory used	50 GB
parallelize	30 nodes



Relative stability of varying hydrogen saturation