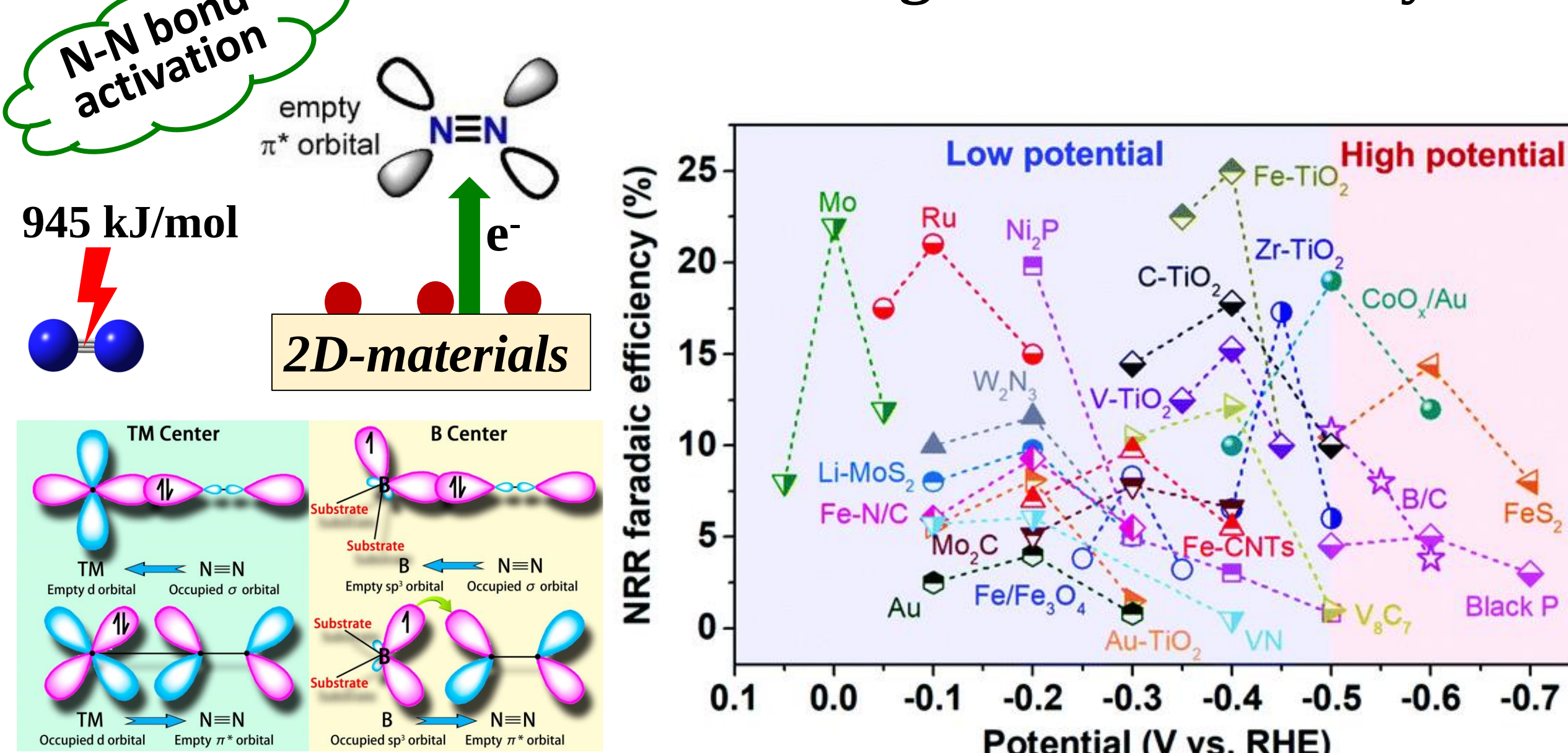


Synopsis

Industrial ammonia production with the Bosch-Haber's method is one of the most energy expensive process that consumes nearly 6% of global energy and releases over 500 million tonnes of CO₂. Considering the multitude and importance of ammonia in agriculture, chemicals and industry; nitrogen fixation at ambient conditions is the need of the hour. The first step to N₂ reduction is the activation of N-N bond, which can be triggered by electron transfer into the antibonding orbital of N₂ molecule. Herein, 2D materials being electron-rich can be employed as electron reservoirs and their inactive basal plane tapped by introducing a metal or non-metal catalytic center. Our DFT driven investigations on earth abundant metal/non-metal anchored 2D materials aim at tailoring cost efficient ambient reduction of nitrogen to ammonia.

Electronic Insights & NRR catalysts



Ling, C.; Niu, X.; Li, Q.; Du, A.; Wang, J. *J. Am. Chem. Soc.* 2018, 140, 43, 14161–14168.
 Ren, Y.; Yu, C.; Tan, X.; Huang, H.; Wei, Q.; Qiu, J. *Energy Environ. Sci.*, 2021, 14, 1176–1193.

Methodology

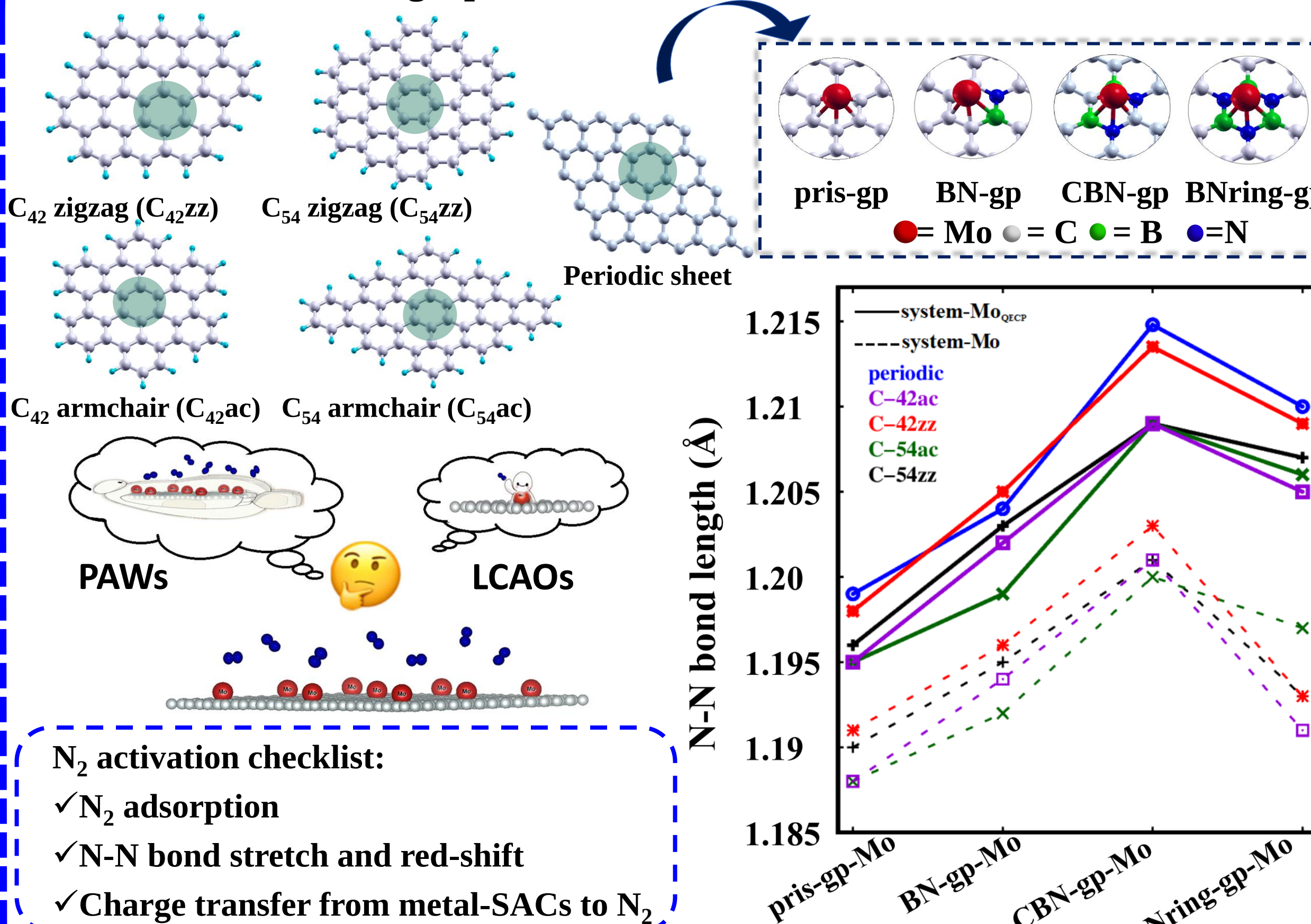
- Schemes:**
1. anchor transition metal (TM) single atom catalysts (SACs) or boron atom catalysts on 2D materials,
 2. synergistic enhancement of catalytic properties by introducing non-metal dopants.

- Density Functional Theory (DFT) calculations
 - Non-periodic DFT: deMon2k - PBE functional with electron implicit & explicit basis sets.
 - Periodic DFT (+D3 correction): VASP - PBE functional with PAW pseudopotentials.

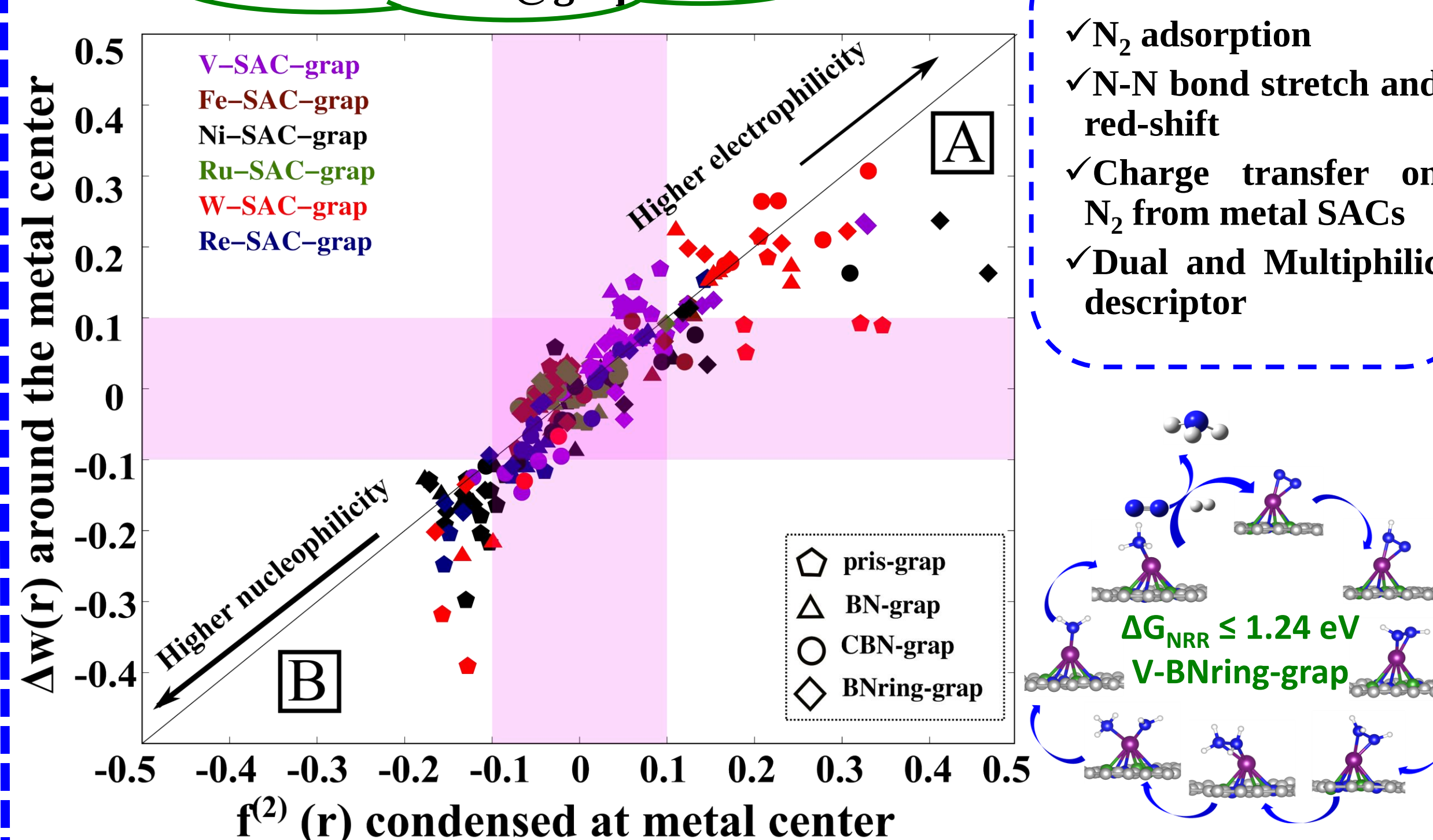


Catalyst 1: M-SAC@BN-doped graphene

Metal SACs anchored graphene models



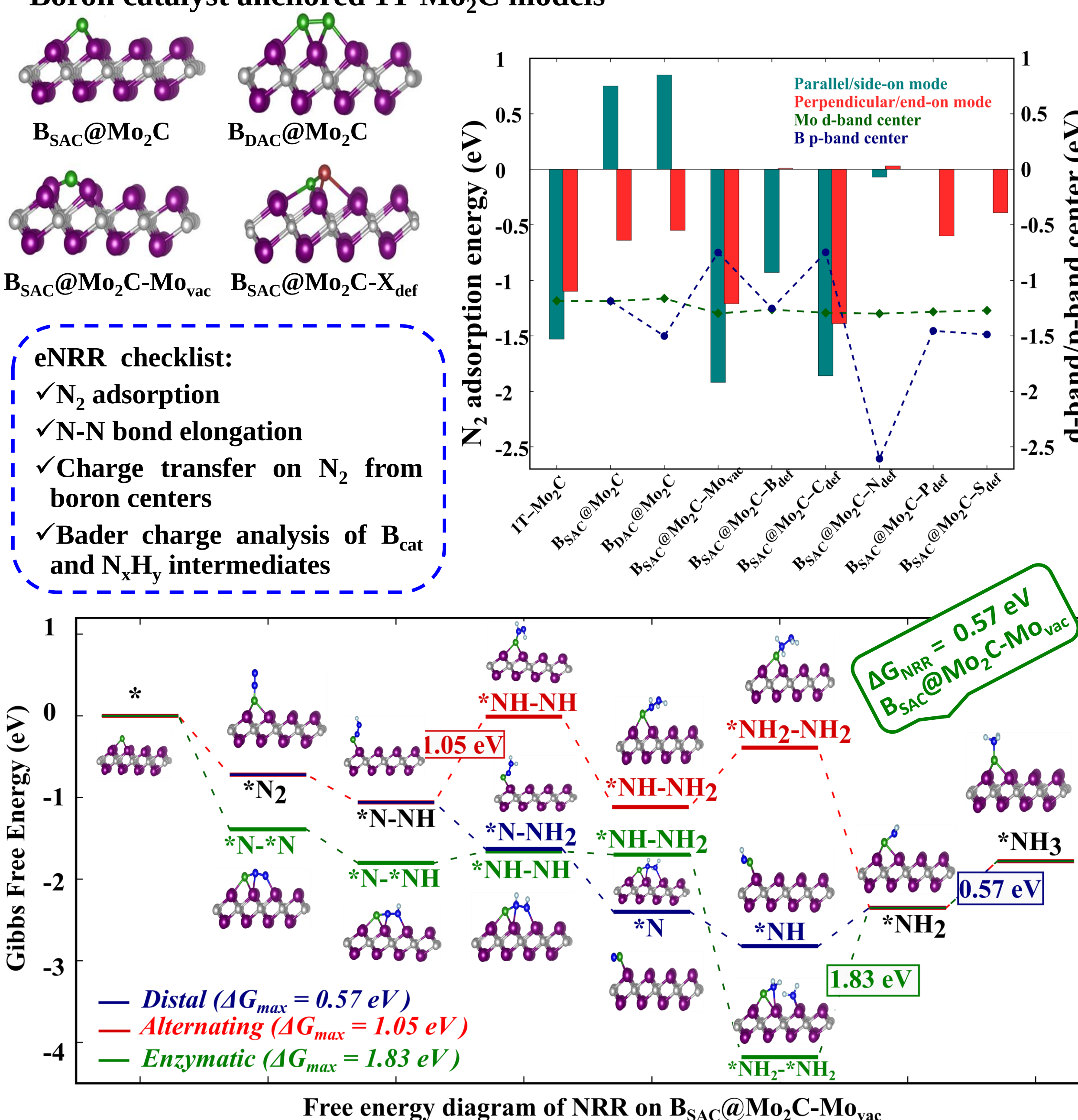
Descriptor based classification of M-SACs@graphene



1. Dinitrogen activation on graphene anchored single atom catalysts: local site activity or surface phenomena. Maibam, A.; Govindaraja, T.; Selvaraj, K.; Krishnamurthy, S. *J. Phys. Chem. C* 2019, 123, 27492–27500.
2. Nitrogen activation to reduction on a recyclable V-SAC/BN-graphene heterocatalyst sifted through dual and multiphile descriptors. Maibam, A.; Krishnamurthy, S. *Journal of Colloid and Interface Science* 2021, 600, 480–491.

Catalyst 2: B_{cat}@Mo₂C (MXenes)

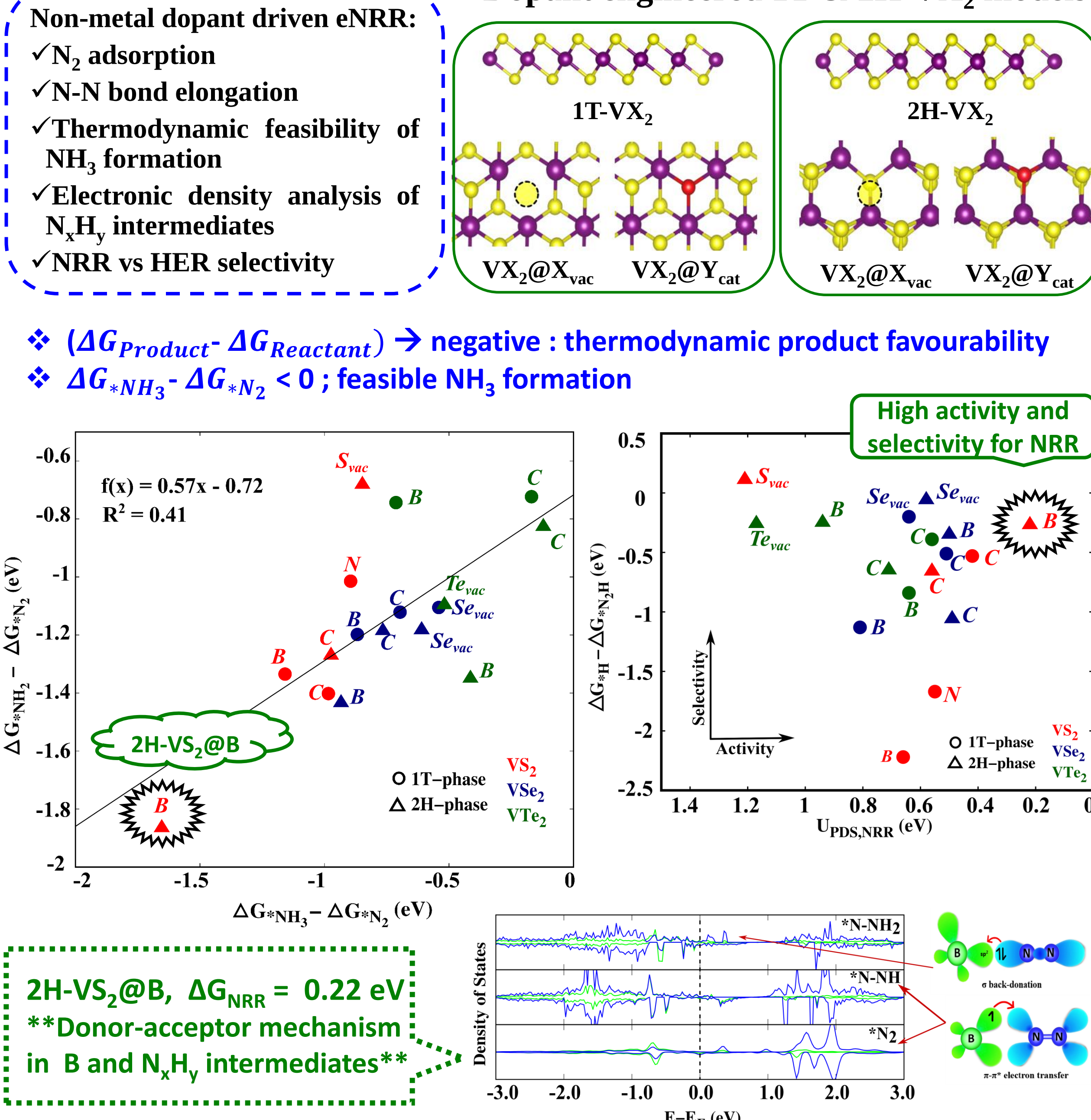
Boron catalyst anchored 1T-Mo₂C models



Electrocatalytic nitrogen reduction directed through the p-band center of boron on B_{SAC}@Mo₂C. Maibam, A.; Krishnamurthy, S.; Dar, M. A. *Mater. Adv.*, 2022, 3, 592–598.

Catalyst 3: Non-metal doped VX₂ (X= S, Se, Te)

Dopant engineered 1T & 2H-VX₂ models



Doped 2D VX₂ (X = S, Se, Te) monolayers as electrocatalysts for ammonia production: A DFT based study. Maibam, A.; Babarao, R.; Krishnamurthy, S.; *Applied Surface Science*, 2022, 602, 154401.

Future Work

