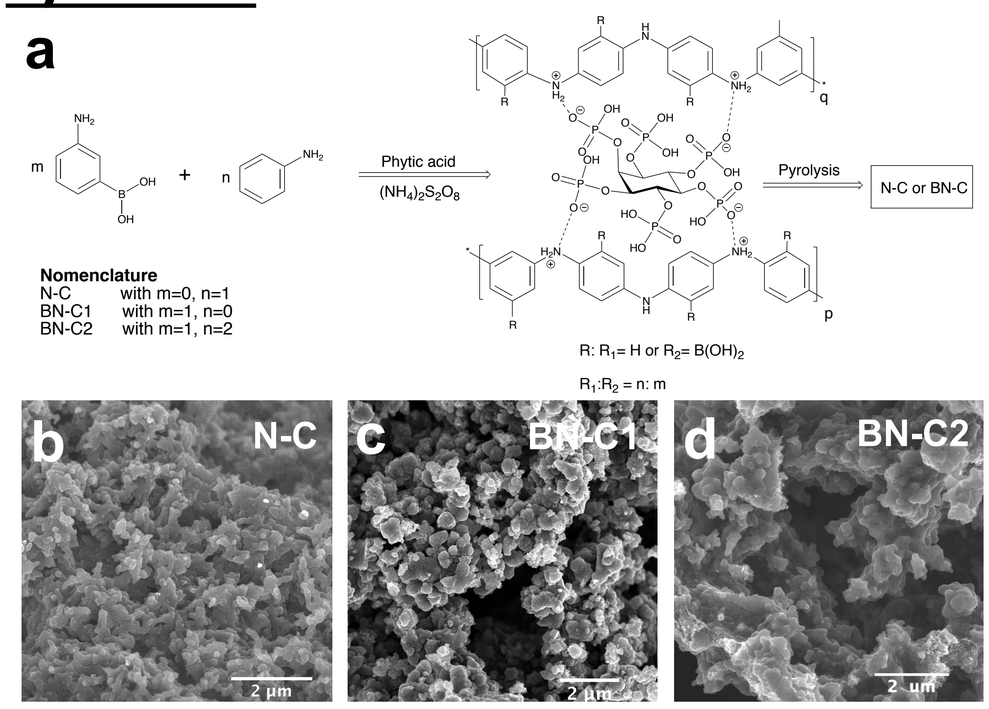
Boron Nitride Islands in Carbon Materials for Efficient Electrochemical Synthesis of Hydrogen Peroxide

Shucheng Chen†, Zhihua Chen†, Samira Siahrostami†, Drew Higgins, Dennis Nordlund, Dimosthenis Sokaras, Taeho Roy Kim, Yunzhi Liu, Xuzhou Yan, Elisabeth Nilsson, Robert Sinclair, Jens K. Nørskov, Thomas F. Jaramillo and Zhenan Bao

Summary

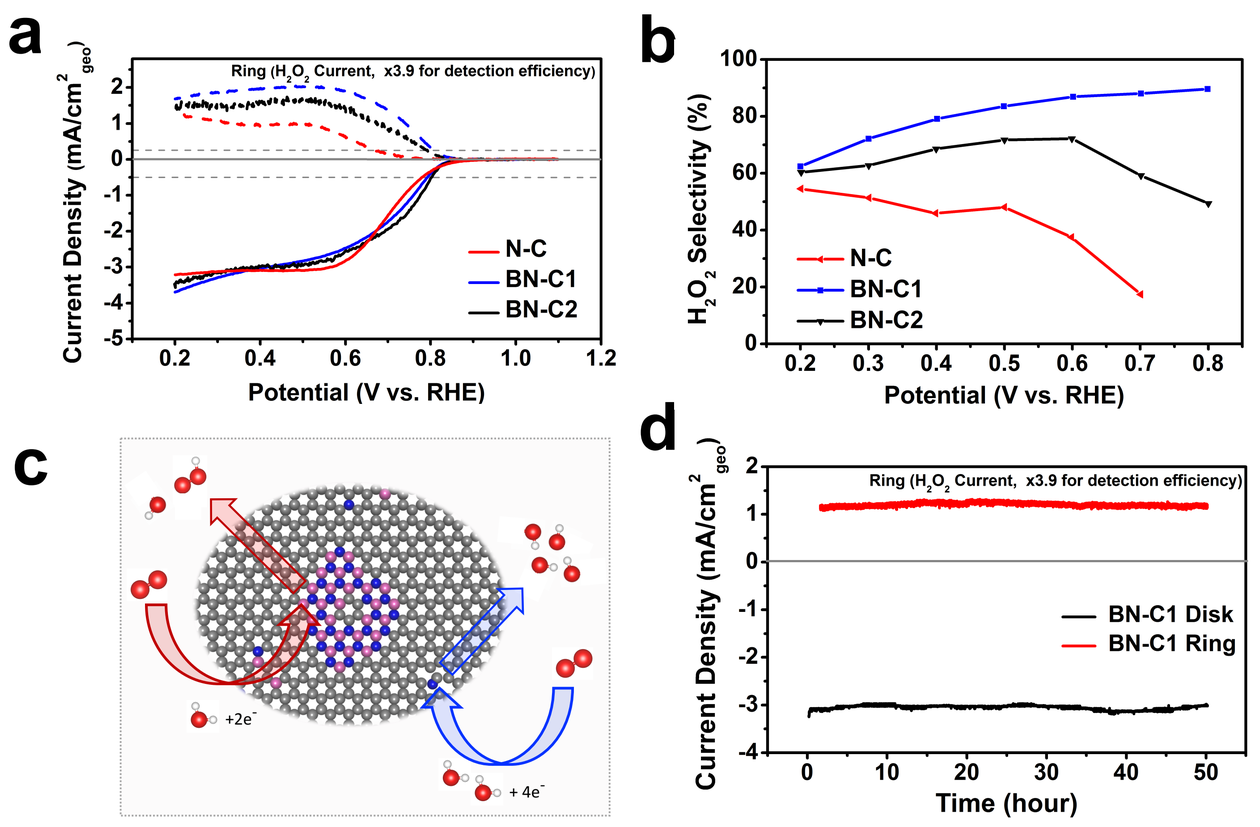
Co-doping of nanostructured carbon with boron and nitrogen has emerged as an attractive strategy to modulate the catalytic activity. However, limited experimental work has been done to systematically study these materials and much remains to be understood about the nature of the active site(s) and the factors underlying the activity enhancements of these boron, carbon and nitrogen (BCN) materials. Herein, we prepared several BCN materials experimentally with a facile method and systematically study their electrochemical performance with controlled synthesis. We demonstrated the existence of *h*-BN domains in the graphitic structure for these materials using x-ray spectroscopy. These synthesized structures yielded higher activity and selectivity toward H_2O_2 than structures with individual B- or N-doping. We further employ density functional theory (DFT) calculations to understand the role of a variety of *h*-BN domains within the carbon lattice for the oxygen reduction reaction (ORR) and find that the interface between *h*-BN domains and graphene exhibits unique catalytic behavior that can preferentially drive the production of H_2O_2.

Synthesis

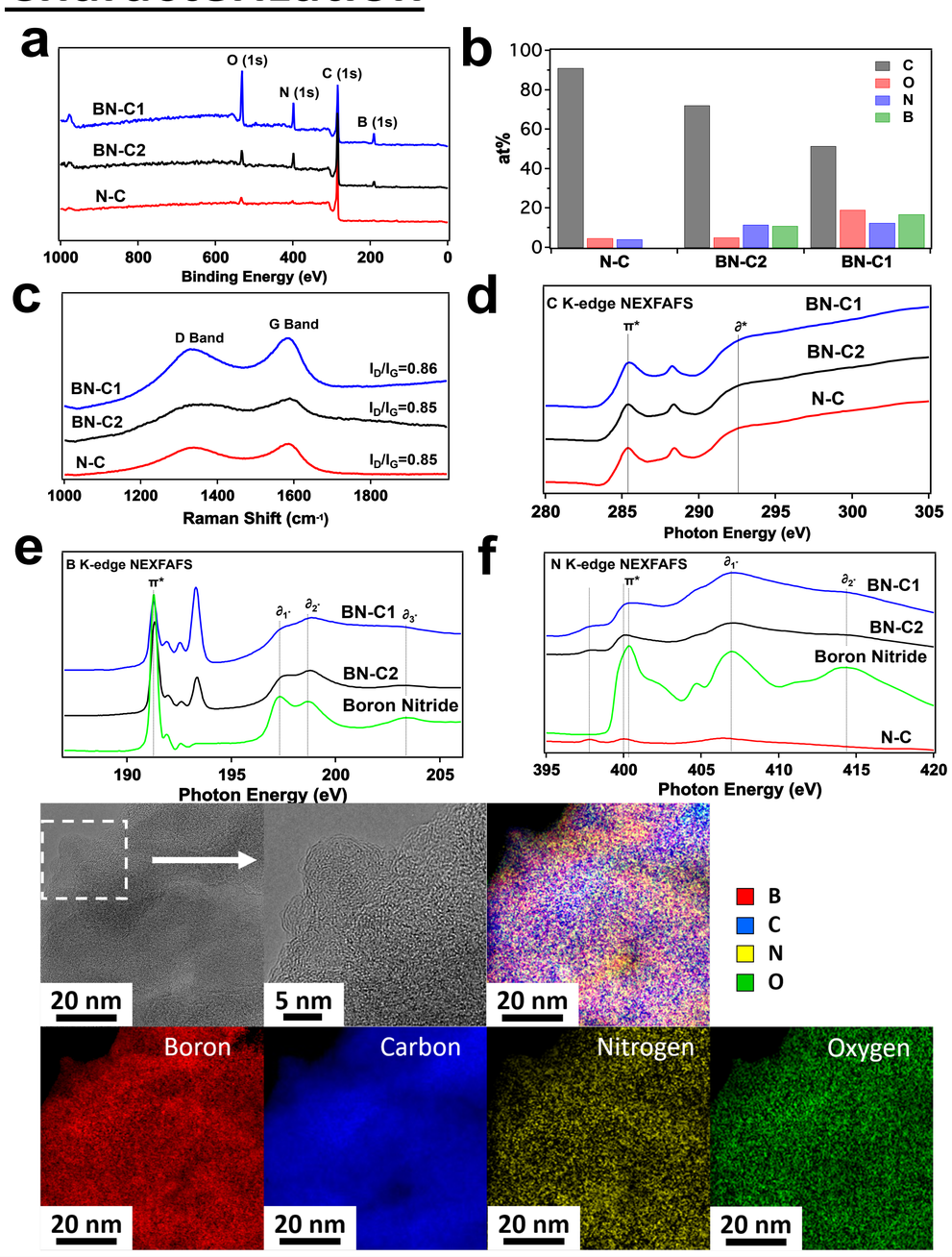


Sample	C (at%)	O (at%)	N (at%)	B (at%)	B and N together in *h*-BN domain (at%)	Single N site (at%)	B in the form of BC_2O (at%)	B in the form of BCO_2 (at%)	BET Surface Area (m^2/g)
N-C	91.1	4.7	4.2	*	*	4.2	*	*	632
BN-C1	51.5	19.2	12.5	16.8	14.5	5.29	0.91	8.64	74
BN-C2	72.2	5.2	11.5	11	10.5	6.23	2.35	3.19	751

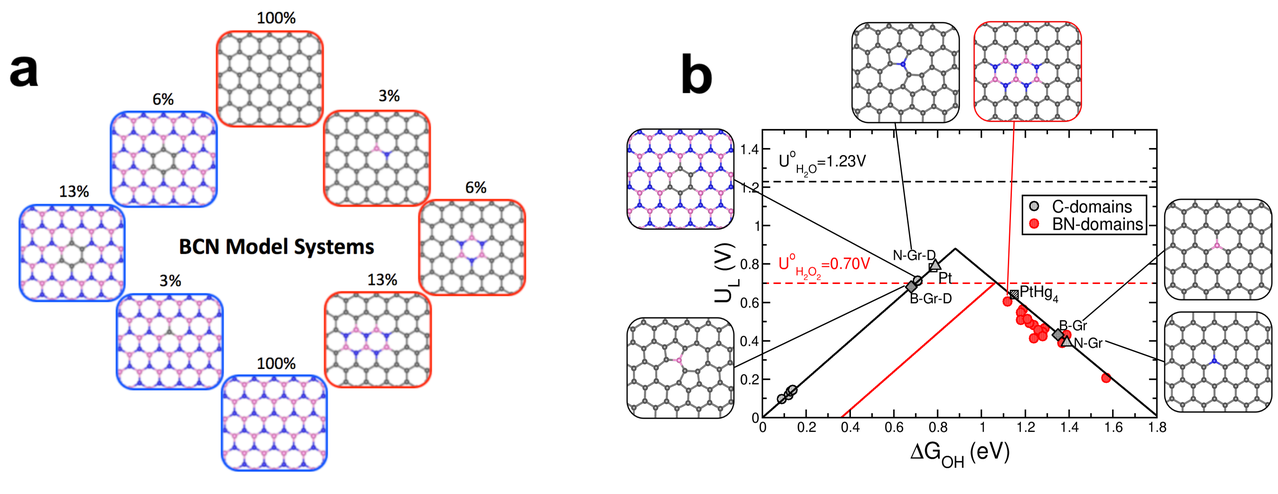
Electrocatalysis Performance



Characterization



Calculations



Applications