

2D Borocarbonitrides: Tunable electronic properties

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Two dimensional materials have received much attention in recent years owing to their fascinating properties in monolayer or few layers. The ability to tune the physical properties by tailoring the electronic structure has always interested researchers. Borocarbonitrides, $B_xC_yN_z$, are 2D materials which allow tuning of electrical and optical properties from high bandgap (~ 5.9 eV) h-BN to low gap of graphene.¹ Thermal properties of BCN are expected to show ultra-low thermal conductivity than its analogues h-BN and graphene.² The electrical and optical behavior was probed by depositing $(BN)_{1-x}(C)_x$ thin films of varied chemical compositions using pulsed laser deposition (PLD) technique, and the thermal property was examined by synthesizing BCN nanosheets by solid-state reaction. Optical and electrical properties of these films show systematic changes in the band gap and the resistivity with composition. The optical and electrical properties of BCN show linear dependence with the composition. BCN nanosheets exhibit p-type semiconducting thermoelectric transport properties, and total thermal conductivity is found to be very low (0.58 to 1.86 W/mK) in 300-573 K range. The ultra-low thermal conductivity and tunable electronic properties of BCN with composition can be shown to have potential applications in thermal management devices and tunable Opto-/nano-electronic devices, respectively, for sustainable future.

References

- (1) Kumar, N.; Moses, K.; Pramoda, K.; Shirodkar, S. N.; Mishra, A. K.; Waghmare, U. V.; Sundaresan, A.; Rao, C. N. R. Borocarbonitrides, $B_xC_yN_z$. *J. Mater. Chem. A* **2013**, *1* (19), 5806-5821.
- (2) Chakraborty, H.; Mogurampelly, S.; Yadav, V. K.; Waghmare, U. V.; Klein, M. L. Phonons and Thermal Conducting Properties of Borocarbonitride (BCN) Nanosheets. *Nanoscale* **2018**, *10* (47), 22148–22154.