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***Ab-Initio* Calculations of the Electronic Properties of Boron Nitride**[1] ANTHONY STEWART, BETHUEL KHAMALA, DANIEL HART, DIOLA BAGAYOKO, Southern University & A&M College — The potential of Boron Nitride (BN) in nanotechnology is tremendous. BN in its bulk form has a wide band gap with excellent thermal and chemical stability. BN structures can be tailored using various techniques in order to obtain desired materials properties. The State-of-the-art Proton Exchange Membrane Fuel Cell (PEMFCs) technology exploits graphitized carbon as a support for platinum-type catalysts. However, some forms of carbon are susceptible to long-term durability issues such as corrosion which is a detriment to fuel cell performance and viability. Novel non-carbon supports such as BN may provide a pathway for addressing the durability and performance issues associated with carbon support materials. We present preliminary theoretical studies, using an linear combination of atomic orbital (LCAO) quantum chemistry package from Ames Laboratory, of the electronic properties of this potentially important material. Our calculated band gap of 6.48 eV for the cubic structure, obtained with an LDA potential and the BZW-EF method, is in agreement with experiment.

[1]LASIGMA/ NNSA_MSIP

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