

# Siemens Competition

## Math : Science : Technology

### Regional Finalist

**Names:** Jesse Cai and Matthew Yu

**High School:** Thomas Jefferson High School for Science and Technology and Montgomery Blair High School

**Mentor:** Dr. Xuan Luo

**Project Title:** *Induced Magnetization and Band Gap in Graphene-Like Materials: Towards Spintronics (Physics)*

We use first principles calculations incorporated within the ABINIT package to analyze the potential of two dimensional graphene-like materials in spintronics. Spintronics has the potential to vastly improve upon and decrease the size of existing silicon based technology. We used three transition metals, Fe, Co, and Ni, to dope four graphene-like materials: graphene, boron nitride, silicene, and molybdenum disulfide. We found that with the addition of certain dopants, configurations involving boron nitride or silicene exhibited magnetization and a band gap in both spin up and spin down channels. Doped graphene showed no band gap, but by using a hybrid graphene/boron nitride surface or by placing graphene on a boron nitride substrate, a band gap was induced in the spin up channel. Similarly, molybdenum disulfide exhibited a band gap in only one of the spin channels. Thus, we conclude that boron nitride and silicene have the most promise in developing spintronic devices, while graphene and molybdenum disulfide can still be incorporated in spin gapless semiconductors.