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Non-Confidential Description - PSU No. 4049**“Controlled Synthesis and Transfer of Large Area Heterostructures Made of Bilayer and Multilayer Transitional Metal Dichalcogenides”****Keywords/Field of Invention:**

Transition Metal Chalcogenide, Heterostructures, Layered Materials, Valley Polarization

Inventor

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Background

Bulk phases of trigonal prismatic transition metal dichalcogenides (TMD) can be semiconducting, metallic, or superconducting, depending on the atomic composition. Recently, it has been found that a monolayer of semiconducting MoS₂, obtained by exfoliation exhibits a direct band gap instead of having an indirect band gap as in the bulk. The importance of having direct band gap is that the material can have optical properties such as photoluminescence at different wavelength ranges and that it also exhibits valley polarization effects. Bulk hexagonal phases of layered semiconducting transition metal dichalcogenides (STMD) such as MoS₂, WS₂, WSe₂, and MoSe₂ exhibit indirect band gaps. Direct band gap has only been known to occur in mono-layered STMDs, which could be used in the construction of optoelectronic devices, catalysts, sensors and valleytronic components.

Invention Description

The Penn State researchers have demonstrated for the first time that it is possible to obtain novel direct band gap bilayers of STMD. By overlapping different monolayers, the resulting bilayers exhibit different behavior from that found for monolayers of STMDs. As documented in the two below referenced papers, the researchers calculated band gaps ranging from 0.8 eV to 1.2 eV. The novel hybrid bilayer systems exhibit new optical properties useful for applications in the infrared range. The researchers have developed four (4) novel families of these hybrid STMDs; each having their own unique optoelectronic properties. The invention's process consists of a two-step thermal reduction sulfurization method to synthesize large areas of these materials with controllable thickness (currently ~ 1 cm²), which is amenable to scale-up, according to the inventors.

Status of Invention

As indicated by the two below-referenced peer-reviewed publications, the invention has experimental results that confirm the theoretical understanding that hetero-layered nanostructures consisting of transition metal dichalcogenides exhibit novel semiconducting properties not seen in homostructures. The inventors continue their government-funded research to test these materials optoelectronic and magnetic properties.

“Controlled Synthesis and Transfer of Large-Area WS₂ Sheets: From Single Layer to Few Layers”, ACS Nano, Vol.7, No. 6, pp 5235-5242, Published online May 6, 2013:

“Novel hetero-layered materials with tunable direct band gaps by sandwiching different metal disulfides and diselenides” by H. Terrones, *et al.*, Scientific Reports, Volume 3: 1549, Published March 26, 2013.

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