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Abstract (Approved for Public Release)

Overview and problem statement: This project will create a new comprehensive research field of one-dimensional (1D) quantum materials consisting of *individual atomic chains* and *few-chain threads* of van-der-Waals (vdW) materials, and composites comprised of bulk polymer matrix with 1D atomic chain fillers. Thereby, it will shift the current paradigm by taking one step down in dimensionality from 2D vdW materials, and creating truly 1D *quantum* materials. The proposed research focuses on unfettered, beyond-conventional approaches to the discovery of materials that exhibit previously unattainable functionalities. Limited experimental work is available only for *bundles* of atomic chains of such 1D vdW materials, suggesting extraordinary electrical current densities and unusual electron-phonon coupling. Computational machine learning studies indicate that there are hundreds of vdW materials with *true*-1D or *quasi*-1D crystalline structures consisting of 1D atomic threads weakly bound in bundles. Exfoliated to a few-chain atomic threads, these materials become genuinely quantum: owing to their atomic scale dimensions and atomically sharp interfaces, the electron states are quantum confined; in addition, many of 1D vdW materials are *strongly-correlated* quantum systems, which reveal non-trivial quantum phenomena, such as charge-density-wave (CDW) condensate phases, magnetic phases, superconductivity, strong spin-orbit coupling, and non-trivial topology.

Project goals and objectives: We propose to perform a comprehensive study of 1D quantum materials with the goals of understanding the limits of downscaling of 1D vdW crystals; fine-tuning electron and phonon transport, quasi-particle interactions; and controlling strongly-correlated quantum phenomena in 1D materials. We anticipate discoveries of unique electronic, thermal, and optical properties of 1D quantum materials, resulting from the ultimate quantum confinement of elemental excitations and collective quantum states. We will apply perspectives from physics, chemistry, materials science and engineering to provide high-payoff research results. Project objectives include: 1) exfoliating 1D vdW materials down to the *ultimate single-atomic chain* limit; 2) determining the electrical, thermal, magnetic, and optical characteristics of 1D materials; 3) establishing the electrical control of these characteristics; and 4) understanding and engineering the properties of *quantum composites* comprised of the polymer matrix and 1D vdW fillers. Innovative technical approaches include nanofabrication of capped and suspended 1D vdW devices to study single quantum phase-slip events; electronic "noise spectroscopy" for monitoring CDW and magnetic phase transitions; Brillouin-Mandelstam-Raman spectroscopy of confined elemental excitations; polarization photoluminescence spectroscopy of excitons; thermal bridge measurements of heat conduction properties; and electromagnetic testing of dielectric constants of composites with 1D vdW fillers. The experimental research will be supported by the world-class *ab-initio* theory.

Anticipated project outcomes and impact on DoD capabilities: The long-term outcomes of this project will create a foundation for the new class of 1D quantum materials and composites based on such materials with numerous potential applications to DoD scientific priorities and operational needs. The proposed 1D vdW quantum materials will lead to revolutionary innovations in the electronics, sensors, and energy conversion, areas which are of importance to DoD. These materials will impact the DoD capabilities in low-power memory and logic, nanoelectronics, antenna design and communications, as well as energy conversion and thermal management. Additionally, this project will educate and train researchers for the defense workforce at a University with a rare combination of being an accredited Hispanic Serving Institution and a highly ranked research-intensive institution.