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Optical and Electronic Properties of Two-Dimensional Materials by Computational Analysis

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Two-dimensional inorganic nanostructures provide a versatile material platform for applications. Here, in the context of algorithm development for modelling periodic material systems on quantum computers, we provide examples of interest, where the optical and electronic properties can be tuned by defects, morphology or incorporation of moieties. We discuss the calculated optical response of transition metal dichalcogenides, specifically monolayer WSe_2 with vacancy defects, which demonstrated promise for single-photon emission. In aiming to achieve a red-shift in the localized excitons, we report on the optical spectra of monolayer WSe_2 with extended patterns, resulting in such a shift. Furthermore, in considering the morphology of the monolayer, such as in generation of wrinkles, the potential for single-photon emission is shown. Next, the role of the organic ligand within the inorganic framework of 2D hybrid organic-inorganic perovskites, proven promising for nonlinear optical applications, will be discussed. Dependent on the organic moiety, band alignments indicate variability in quantum-well types and absorption spectra, motivating further synthesis and experimental characterization. Finally, we describe the electronic properties of patterned graphene, fabricated using electron-beam chemistry with radiolyzed water vapor. Calculated defect-induced Raman intensities demonstrate consistency with experimental data, and electron transport calculations of alternating pristine and epoxide defective strips in graphene demonstrate comparable characteristics to graphene nanoribbons.

Dr. Ruth Pachter is a member of the scientific and technical cadre of senior executives, appointed in 2001 as a senior scientist at the Air Force Research Laboratory, Materials and Manufacturing Directorate. She joined the Materials Directorate in 1991 from Stanford University. In 1994, she was appointed a physical scientist at the National Institute of Standards and Technology, co-located at Wright Laboratory, and in 1997 became a principal physical scientist in AFRL. Dr. Pachter received her undergraduate degree in chemistry and physics from the Hebrew University, Israel, and graduate degrees in theoretical chemistry from the Technion, Israel Institute of Technology, and the University of South Africa. Dr. Pachter's research interests center on computational chemistry and materials science, with application to optical and electronic materials that address Air Force needs. Dr. Pachter is author and co-author of more than 170 refereed publications, served on journal editorial boards, and is active in professional societies.

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