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One-dimensional van der Waals materials—Advent of a new research field

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Alexander A. Balandin,[1,a] Roger K. Lake,[1] and Tina T. Salguero[2]

AFFILIATIONS

[1]Department of Electrical and Computer Engineering, Materials Science and Engineering Program, University of California, Riverside, California 92521, USA

[2]Department of Chemistry, University of Georgia, Athens, Georgia 30602, USA

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[a]**Author to whom correspondence should be addressed:** balandin@ee.ucr.edu

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Investigations of the unique electrical, thermal, and optical properties of graphene have generated tremendous progress in fundamental and applied sciences.[1–5] The advent of graphene stimulated the search for other two-dimensional (2D) van der Waals atomic crystals with properties distinct from their corresponding bulk forms. A large number of materials in the family of transition metal dichalcogenides (TMDs) have weak van der Waals bonding between 2D structural units, allowing for exfoliation to quasi-2D layers. Other, less well-researched classes of van der Waals materials have one-dimensional (1D) or quasi-1D structural units.[6–15] Some of these, like $TaSe_3$, are quasi-1D in the sense that they have strong covalent bonds in one direction along the atomic chains and weaker bonds in the perpendicular plane.[8] Other materials, like $ZrTe_3$, can be considered intermediate 2D/1D-type based on structure and properties.[11,16] Yet, others are best considered true-1D materials; these have covalent bonds only along the atomic chains and much weaker van der Waals interactions in perpendicular directions.[16] We consider both quasi- and true-1D examples to be "1D materials," especially if they are exfoliated or grown into individual atomic chains or atomic threads comprising just a few chains. It is important to note that the true- and quasi-1D van der Waals materials are fundamentally different from "nanowires" or "quantum wires"—understood to be nanostructures of conventional covalent or ionic semiconductors or metals. Such nanowires have larger diameters and lack the atomically sharp interfaces of van der Waals materials. Furthermore, owing to their crystal structures, covalent nanowires cannot be downscaled to individual atomic chains.

Machine learning studies suggest the existence of hundreds of 1D van der Waals materials with bandgaps ranging from metallic to insulating.[18] One prominent group is the transition metal trichalcogenides (TMTs) with the formula MX_3 (where M = Mo, W, etc.; X = S, Se, Te). In the monoclinic crystal structure of $TaSe_3$, for example, the trigonal prismatic $TaSe_3$ units form continuous chains extending along the *b*-axis and creating needlelike crystals.[8,17] The TMT crystals exfoliate into chain structures, unlike TMDs that exfoliate into atomic planes. It is feasible that van der Waals crystals can be exfoliated or grown into atomic chains with cross-sectional dimensions of $\sim 1 \times 1\ nm^2$.[16,19,20] The first studies of the exfoliated metallic TMT bundles discovered exceptionally high breakdown current densities in such materials, exceeding those in Cu and other elemental metals by more than an order of magnitude.[8,11,16] A key characteristic of 1D van der Waals bundles or chains is that they can be well-ordered, single-crystalline, in one direction, and have few or no dangling bonds. Some of these materials have revealed unusual properties related to strongly correlated quantum phenomena, e.g., charge density waves and topological effects.[16] Related work has demonstrated that composites with fillers comprised of 1D van der Waals materials have exceptional electromagnetic shielding efficiency.[21,22] These recent developments suggest that continued reduction in dimensionality to individual atomic chains can bring exciting prospects at the ultimate limit of material downscaling. This perspective motivated this timely Special Topic Issue with contributions focused on developments related to one-dimensional van der Waals materials.[23–40]

As an entirely new field, one-dimensional van der Waals materials encompass interdisciplinary work by physicists, chemists, materials scientists, and engineers. Therefore, the contributions in the Special Topic Issue span theoretical and computational developments pertinent to the prediction of the stable structures of such materials and their electronic and magnetic properties, as well as experimental studies that illustrate their preparation, properties, and prospects for practical applications.[23–40] The 1D materials investigated include TMTs like TiS_3, $ZrTe_3$, and NbS_3;[25,27,29–31,37] other metal chalcogenide compositions like Ta_2Se_3 and $Ta_2Ni_3Se_8$;[33–35] emerging classes of 1D

materials like metal halides, e.g., $OsCl_4$ and Bi_4Br_4, and chalcohalides, e.g., $(TaSe_4)_2I$ and BiSeI;[23,24,28,32,36,40] and additional 1D systems ranging from elemental selenium to covalent organic framework-carbon nanotube heterostructures.[26,38,39] Synthetic studies cover preparative techniques, such as alloying, doping, and exfoliation,[29,33,35] as well as structural studies that demonstrate lattice engineering and clarify issues of polymorphism.[29,33]

Specific contributions illustrate an ongoing research related to the properties of 1D van der Waals materials. The electronic and magnetic properties of 208 transition metal dihalide and trihalide nanowires are described in Ref. 23; a detailed account of the electronic and magnetic properties of $OsCl_4$ is provided in Ref. 24. Four papers focus on TiS_3 and its electronic, energy-storage, photonic, and piezoelectric properties.[27,30,31,37] Its high-electric-field behavior and possible metal–insulator transition are experimentally analyzed in Ref. 37. The photoconductivity of TiS_3, measured over the temperature range of 5 to 300 K, is used to characterize the nature of possible phase transitions to the collective states in Ref. 30. The measured anisotropic piezoresistance of TiS_3 is found to have opposite signs when tensile strain is applied along the chains or perpendicular to the chains;[27] a high specific capacitance is measured for TiS_3 used as a positive electrode in a supercapacitor device.[31] Several contributions focus on optoelectronic properties. It was found that the photo-response of BiSeI is significantly enhanced in mechanically exfoliated thin wires compared to that of the bulk.[28] The predicted 1D topological insulator Bi_4Br_4 can be used as a saturable absorber integrated with a laser allowing mode-locking at the near-infrared with sub-picosecond pulse duration.[36] Recently, there was considerable excitement over possible strong longitudinal magnetoresistance interpreted as evidence of axionic charge density waves in $(TaSe_4)_2I$. This issue is addressed in Ref. 40. Different physical mechanisms are discussed, and further experiments are proposed to probe the nature of the charge density wave state in $(TaSe_4)_2I$. This brief recount of the intriguing properties of 1D van der Waals materials should provide sufficient motivation for further browsing and perusal of this Special Topic Issue by interested readers.

In conclusion, this Special Topic Issue provides a glimpse of new, vibrant, and innovative research associated with 1D van der Waals materials. These contributions are defining this new field as it materializes from long-standing, broader interest in low-dimensional systems. Exciting progress is happening at a rapid pace, and we anticipate that this Issue will be relevant and interesting for many researchers.

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AUTHOR DECLARATIONS

Author Contributions

Alexander A. Balandin: Conceptualization (equal). **Roger K. Lake:** Conceptualization (equal). **Tina T. Salguero:** Conceptualization (equal).

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