# Two-Dimensional Charge-Density-Wave Materials with Unique Advantages for Electronics

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## Abstract
Two-dimensional (2D) charge density wave (CDW) materials have attracted widespread attention due to their exotic physical properties. Compared to their bulk forms, 2D CDW materials exhibit many excellent features, offering new possibilities for electronic device applications. In this Perspective we highlight the unique advantages of 2D CDW materials and identify some key challenges which remain to be addressed.

**Key words:** Charge density wave; Two-dimensional materials; Transition metal dichalcogenides; Dimensionality effects

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## Main text

A charge density wave (CDW) phase is a broken-symmetry state where the charge density acquires a periodic modulation and the atomic lattice is periodically distorted[1,2]. It has long been a research hotspot because of its fascinating physical properties and great application potential in electronic devices such as oscillator and memory[3–7]. Many layered transition metal dichalcogenides (TMDCs) including 1T-$TaS_2$, 2H-$NbSe_2$, 1T-$TaSe_2$ and so on are prototypical CDW materials [8,9]. For example, 1T-$TaS_2$ undergoes a series of first-order phase transitions from the high-symmetry 1T phase to $\sqrt{13} \times \sqrt{13}$ CDW phase with decreasing of temperature, which is considered to be an ideal candidate for applications of devices due to its tunable CDW phases[10–18]. In recent years, with the rapid advances in fabrication technologies of two-dimensional (2D) materials, particular attention has been paid to the CDW phases in 2D materials[19–21]. To date, CDWs have been observed down to the monolayer limits of some TMDCs[22–25]. Due to the reduced dimensionality, the 2D CDW phases show many different features compared with their bulk counterparts, which makes them have unique advantages over the three-dimensional (3D) CDW phases in some respects.

First, it was reported that lowering dimensionality is able to increase the CDW transition temperature ($T_{CDW}$) below which the CDW phase survives. Most of the CDW phase transitions in the bulk TMDCs occur at very low temperatures, making the application very cumbersome. Therefore, increasing $T_{CDW}$ is a desirable goal. Xi *et al.* observed $T_{CDW}$ of 2H-$NbSe_2$ strikingly increases from 33 K in the bulk sample to 145 K in the monolayer, with the 3 × 3 CDW order persisting[9]. By first-principles calculations, Lian *et al.* further revealed that the cost of the lattice elastic energy by the CDW distortions is greatly reduced in monolayer 2H-$NbSe_2$ due to the absence of interlayer coupling, resulting in the increase of $T_{CDW}$[26]. It was also found that single-layer 1T-$TiSe_2$ shows a 2 × 2 CDW transition at $T_{CDW}$ = 230 K, which is higher than the bulk $T_{CDW}$ = 200 K[27].

Second, because of the dramatic reduction of electronic screening, 2D CDW phases usually exhibit exotic quantum phenomena that are not found in their bulk phases. Take 1T-$TaSe_2$ as an example. At room temperature, bulk 1T-$TaSe_2$ is stabilized in a commensurate $\sqrt{13} \times \sqrt{13}$ CDW phase and shows metallicity[28,29]. In the monolayer limit, the $\sqrt{13} \times \sqrt{13}$ CDW phase is also observed. However, the strong electron correlations make it become a Mott insulator with unusual orbital texture[30]. It is also worth noting that the CDW-Mott insulator transition temperature of monolayer 1T-$TaSe_2$ is as large as 530 K, which is favorable to the realization of CDW-Mott insulator-based ultrathin nanoelectronic devices operating at room temperature[31].

In some materials, the reduced dimensionality even changes the periodicity of the CDW order. It was experimentally reported that single-layer 1T-$VSe_2$ displays a $\sqrt{7} \times \sqrt{3}$ CDW phase in sharp contrast to the 4 × 4 CDW phase in the bulk, with its $T_{CDW}$ of 220 K being twice of the bulk value[32,33]. In addition, bulk 2H-$NbS_2$ displays no CDW due to strong anharmonicity, while freestanding 2H-$NbS_2$ monolayer is reconstructed into an interestingly quantum enhanced 3 × 3 CDW phase in the 2D limit[34,35]. Recently, monolayer 1T-$NbTe_2$ was also predicted to have a 4 × 4 stripe-like CDW phase which is completely different from the bulk 3 × 1 CDW phase[36,37]. The new emerging CDW orders in the 2D limit endow more pos-

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sibilities of finding novel properties. For instance, both the quantum spin Hall state and the quantum anomalous Hall state can be achieved in the $4 \times 4$ CDW phase of monolayer 1T-$NbTe_2$, depending on the choice of the substrate[37].

Third, 2D CDW phases can be easily modulated by external stimuli due to their atomically thin structures and high surface-to-volume ratios. The electrostatic gating that can realize electrically tunable doping level of up to $10^{14}$ electrons/holes per square centimeter in ultrathin 2D materials and the external strain that can be controllably introduced into 2D materials by various methods such as piezoelectric stretching have been proved as two effective means of modulating the 2D CDW phases[30,38–40]. Kolekar *et al.* demonstrated that electron doping will suppress the CDW phase in monolayer 1T-$TiSe_2$, inducing an electronic phase transition from a semiconducting to a metallic state[41]. Zhang *et al*. found that when an in-plane compressive strain is applied to the CDW phase of monolayer 1T-$TaSe_2$, it will induce a continuous Mott insulator to charge-transfer insulator and to metal phase transition[30]. The Mott insulator-to-metal transition can also be realized in ultrathin 1T-$TaS_2$ via the $\sqrt{13} \times \sqrt{13}$ C (commensurate) CDW-NC (nearly commensurate) CDW phase transition driven by strain or DC current [42,43]. In addition, varying charge screening of the 2D materials by the underlying substrate also enables the control of CDW. A substantial increase in $T_{CDW}$ of ≈ 45 K was observed in monolayer 1T-$TiSe_2$ on $MoS_2$ compared to that on graphite[41]. It is anticipated that the controllability of 2D CDW phases could open new venues for designing future devices.

In conclusion, compared to their bulk forms, 2D CDW phases have exhibited excellent properties such as higher phase transition temperatures, more exotic electronic properties and better tunability, etc. (see Figure 1), with tremendous promise for applications in fast and efficient memory, sensing and computing devices. Although recent few years have witnessed many breakthroughs in the 2D CDW field, several challenges remain. (i) The formation mechanisms of 2D CDW, and the interplay between 2D CDW and related quantum states including superconductivity, Mott insulators, and topological states are still not clear. (ii) The 2D CDW materials studied now are limited to some TMDCs members, and there is a plenty of room for search and investigation of more 2D materials with CDW. (iii) Developing effective strategies for targeted modulation of 2D CDW phases are indispensable, in order to satisfy the requirements of specific applications. To address these challenges, synergistic efforts from experiments and theory are highly required. It is believed that 2D CDW phases will play a crucial role in the development of the new generation of electronic devices.

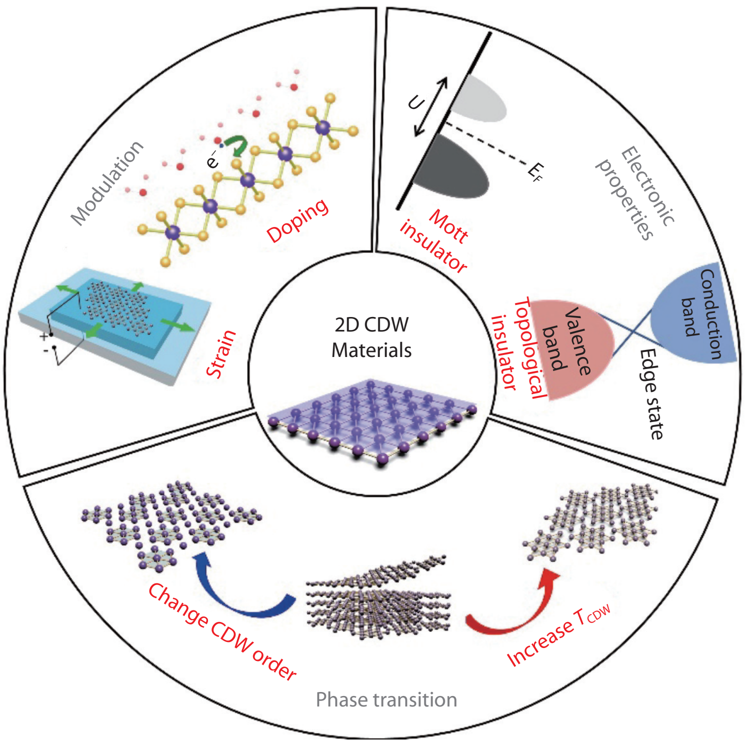


**Fig. 1** Schematic of the unique advantages of 2D CDW materials for electronic device applications. Compared to their bulk forms, 2D CDW materials can exhibit higher phase transition temperatures and more exotic electronic properties such as Mott insulators and topological insulators. They can also be easily modulated by various methods such as strain and doping[30,32,37].

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## Conflict of interest

The authors declare no conflict of interest.

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