

First-principles design of Goldene as efficient two-dimensional metal contact for Janus MoSSe-based heterostructures

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Abstract. Two-dimensional (2D) metal-semiconductor heterostructures play a critical role in determining contact resistance, charge injection efficiency, and overall performance of next-generation nanoelectronic devices. In this work, we computationally design a novel metal-semiconductor Goldene/Janus MoSSe heterostructure and systematically investigate its structural stability, electronic properties, interfacial charge transfer, and contact characteristics by using first-principles calculations. Our results demonstrate that the Goldene/Janus MoSSe heterostructure is energetically favourable and thermodynamically stable, with equilibrium configurations dominated by weak van der Waals interactions that preserve the intrinsic electronic properties of the constituent monolayers and facilitate experimental fabrication. Charge density difference and electrostatic potential analyses reveal pronounced interfacial charge redistribution, with electrons transferred from the Goldene layer to the MoSSe layer in both stacking configurations. As a result, a *p*-type Schottky contact is formed, with Schottky barrier heights of 0.57 and 0.67 eV for the Goldene/SMoSe and Goldene/SeMoS configurations, respectively. These findings highlight Goldene as a promising 2D metal electrode and provide fundamental insights for optimising contact engineering in Janus MoSSe-based nanoelectronic devices.

Keywords: 2D Goldene, metal-semiconductor heterostructure, first-principles calculations, Schottky contact

1 Introduction

Two-dimensional (2D) materials [1] have attracted enormous interest since the successful isolation of graphene [2], whose exceptional electrical, mechanical, and thermal properties demonstrated the transformative role of reduced dimensionality in materials science. Following graphene, a broad family of 2D materials has been developed, including transition metal dichalcogenides (TMDs) [3], MXenes [4], black phosphorus [5], and layered metal oxides [6], encompassing metallic, semiconducting, and insulating behaviours within atomically thin limits. These materials offer outstanding advantages for nanoelectronic and

optoelectronic applications, such as excellent electrostatic control, mechanical flexibility, and the ability to form van der Waals heterostructures without lattice-matching constraints. Nevertheless, the practical implementation of 2D materials remains challenging because of several intrinsic limitations. Graphene, for instance, lacks an intrinsic band gap, which severely restricts its application in logic devices [7], while numerous semiconducting 2D materials suffer from moderate carrier mobility [8]. As a result, there is a pressing need to explore new 2D materials with engineered electronic structures and improved interfacial properties. Designing metal-semiconductor heterostructures has emerged as an effective

approach to overcome the limitations of individual 2D materials by enabling control over band alignment and carrier injection. In particular, van der Waals (vdW) heterostructures formed from 2D metals and semiconductors can provide clean, atomically sharp interfaces and reduced Fermi-level pinning. To date, numerous 2D metal-semiconductor vdW heterostructures have been experimentally realised and theoretically proposed, such as NbS₂/MoS₂ [9], MoSH/GaN [10], MoO₂/MoSe₂ [11], and graphene/TMDs [12] heterostructures. These studies reveal that vdW metal-semiconductor heterostructures provide a versatile platform for tailoring interfacial electronic properties. For instance, Kang et al. [11] demonstrated that a Schottky diode based on the MoO₂/MoSe₂ metal-semiconductor heterostructure exhibits an excellent photovoltaic effect, with a high open-circuit voltage of 0.26 eV and an ultrafast photoresponse. This remarkable performance originates from the naturally formed metal-semiconductor contact with a suppressed Fermi-level pinning effect at the vdW interface. Therefore, systematic investigation of 2D metal-semiconductor heterostructures is essential for the development of high-performance nanoelectronic and optoelectronic devices.

Recently, a novel 2D material, namely, Janus MoSSe, has been successfully fabricated by using several techniques such as plasma-assisted chalcogen substitution and chemical vapour deposition, enabling controlled replacement of one chalcogen layer in conventional TMDs [13, 14]. Owing to its broken out-of-plane symmetry, Janus MoSSe exhibits an intrinsic dipole moment and a built-in electric field, leading to unusual electronic and optical properties. These characteristics make it highly promising for applications in nanoelectronics, optoelectronics, piezoelectric devices, and photocatalysis [15, 16]. Similarly, the recent synthesis of Goldene, a novel 2D material, has broadened the scope of low-dimensional

systems and intensified interest in 2D metals [17]. A Goldene monolayer has been experimentally obtained by selectively exfoliating it from the layered TiAuC precursor, and theoretical studies have confirmed its thermal and mechanical stability under ambient conditions [18, 19]. These features make Goldene a promising 2D metal for integration with other 2D semiconductors.

In this work, we computationally design a novel metal-semiconductor Goldene/Janus MoSSe heterostructure and systematically investigate its electronic properties, contact characteristics and interfacial charge transfer. These results provide fundamental guidance for optimising contact properties in next-generation nanoelectronic devices.

2 Computational methods

All calculations in this work were carried out within the framework of density function theory (DFT) as implemented in the Quantum ESPRESSO package [20]. The exchange-correlation interactions were described by using the generalised gradient approximation in the form of the Perdew-Burke-Ernserhof functional. The Brillouin zone was sampled by using Monkhorst-Pack k-point meshes sufficiently dense to ensure convergence of total energies and electronic properties. A vacuum layer of 30 Å was introduced along the out-of-plane *z* direction to eliminate spurious interactions between periodic images. All atomic structures were fully relaxed until the residual forces on each atom were below a given threshold, and the total energy difference between successive self-consistent steps was converged. A dipole correction was applied in all calculations to eliminate the artificial electrostatic interactions arising from the periodic boundary conditions along the out-of-plane direction. The dynamical stability of the proposed structures was examined by calculating the phonon dispersion spectra using

density functional perturbation theory. *Ab initio* molecular dynamics (AIMD) simulations were performed within the canonical ensemble, employing the Nosé-Hoover thermostat.

3 Results and discussion

The atomic structures of the Goldene/Janus MoSSe heterostructure are depicted in Fig. 1. Owing to the broken out-of-plane symmetry of the Janus MoSSe monolayer, two distinct stacking configurations can be constructed, namely, Goldene/SMoSe and Goldene/SeMoS heterostructures. In the Goldene/SMoSe heterostructure, the Goldene layer is stacked on top of the S-terminated surface of the Janus MoSSe monolayer, whereas in the Goldene/SeMoS heterostructure, the Goldene layer is stacked on the Se-terminated surface. After full structural relaxation, the equilibrium interlayer

distances d between the Goldene layer and the S- and Se-terminated surfaces of the Janus MoSSe monolayer are 3.00 and 2.89 Å, respectively. These interlayer separations are noticeably smaller than those reported for Goldene/MoS₂ ($d = 3.52$ Å) and Goldene/MoSe₂ ($d = 3.45$ Å) [21], indicating a stronger interfacial interaction in the Goldene/Janus MoSSe system. This enhancement can be attributed to the out-of-plane built-in dipole of the Janus MoSSe monolayer, which strengthens the vdW coupling and reduces the equilibrium interlayer spacing. In addition, these interlayer distances are comparable with those reported for the Janus MoSSe-based vdW heterostructures, including Ta₂B/MoSSe [22], NbS₂/MoSSe [23] and graphene/MoSSe [24], indicating that the Goldene and Janus MoSSe layers are bonded together via the weak vdW interactions rather than the strong covalent bonds.

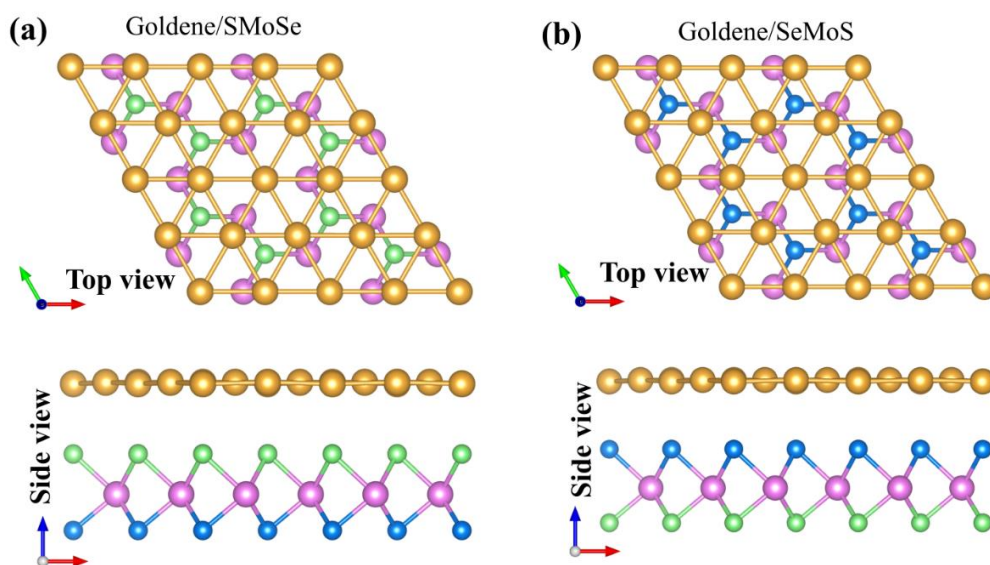


Fig. 1. Top view and side view of relaxed atomic structures of Goldene/Janus MoSSe for two different stacking configurations of (a) Goldene/SMoSe and (b) Goldene/SeMoS. Yellow balls stand for the Au atoms in Goldene, while green, purple and blue balls represent S, Mo and Se atoms in Janus MoSSe layer, respectively.

Furthermore, we evaluate the stability of such heterostructures by calculating the binding energy, performing the AIMD simulations and phonon spectrum of both the Goldene/SMoSe and Goldene/SeMoS heterostructures. The binding energy is obtained as $E_b = [E_{\text{Goldene/MoSSe}} - E_{\text{Goldene}} -$

$E_{\text{MoSSe}}]/A$, where $E_{\text{Goldene/MoSSe}}$, E_{Goldene} , and E_{MoSSe} represent the total energies of the Goldene/MoSSe heterostructure, isolated Goldene and Janus MoSSe monolayers. A stands for the surface area of the heterostructure. The binding energies of the Goldene/SMoSe and Goldene/SeMoS

heterostructures are -44.18 and -41.46 meV/Å², respectively. The negative binding energies indicate that both heterostructures are energetically stable. Moreover, these binding energy values are comparable with those of

graphite [25], confirming that the interfacial interaction is dominated by van der Waals forces and suggesting good feasibility for experimental realisation.

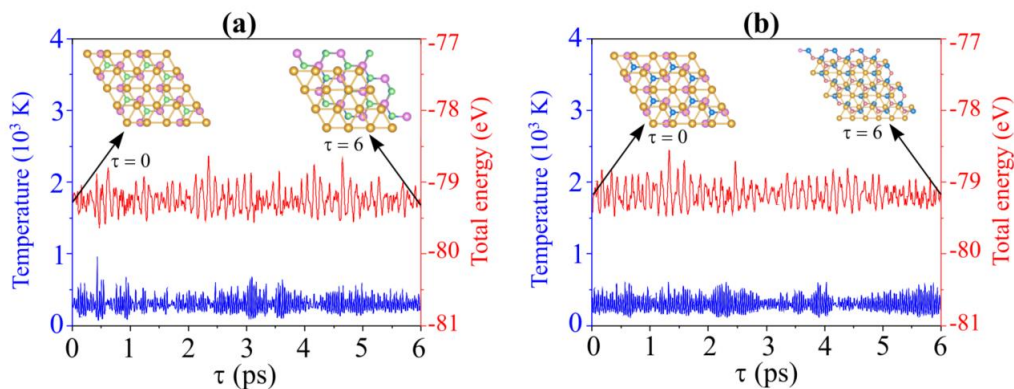


Fig. 2. Fluctuations of temperature and total energy as function of simulation time for (a) Goldene/SMoSe and (b) Goldene/SeMoS heterostructures obtained from *ab initio* molecular dynamics simulations. The insets show the atomic configurations of the heterostructures before and after the AIMD simulations.

The thermal stability of the Goldene/SMoSe and Goldene/SeMoS heterostructures is evaluated by performing AIMD simulations, as illustrated in Fig. 2. The AIMD simulations are carried out at 300 K with a time step of 1 fs for a total simulation time of 6 ps. During the simulation process, both the temperature and total energy exhibit only small fluctuations around their equilibrium values, and no structural reconstruction or bond breaking is observed. Furthermore, the final atomic configurations remain nearly identical to the initial ones, indicating that both heterostructures possess good thermal stability at ambient temperature. In addition to thermal stability, the dynamical stability of the Goldene/SMoSe and Goldene/SeMoS heterostructures is investigated by calculating their phonon dispersion relations, as shown in Fig. 3. One can find that no imaginary phonon modes appear throughout the entire Brillouin zone for either heterostructure, indicating their excellent dynamical stability. The acoustic phonon branches exhibit the expected linear behaviour near the Γ point, while the optical modes remain well separated and free of soft

modes. These results confirm that both heterostructures are dynamically stable and can exist as robust two-dimensional systems.

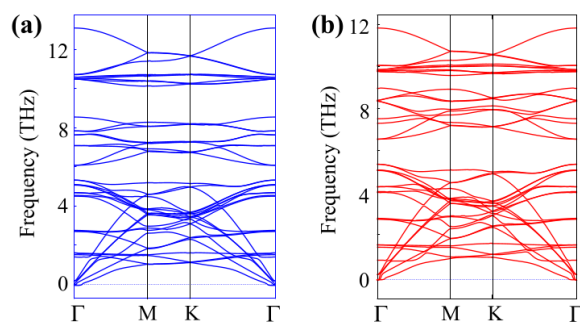


Fig. 3. Phonon dispersion relations of (a) Goldene/SMoSe and (b) Goldene/SeMoS heterostructures calculated along high-symmetry directions of the two-dimensional Brillouin zone

Having confirmed both the thermal and dynamical stability of the Goldene/SMoSe and Goldene/SeMoS heterostructures through AIMD simulations and phonon dispersion analyses, we now turn to their electronic properties. In particular, the projected band structures are calculated to elucidate the interfacial electronic coupling and the contributions of individual layers

to the electronic states near the Fermi level (Fig. 4). It is obvious that the band structures of the Goldene/SMoSe and Goldene/SeMoS heterostructures can be regarded as a superposition of those of the isolated Goldene and Janus MoSSe monolayers. This indicates that the intrinsic electronic characteristics of each constituent Goldene and Janus MoSSe monolayer are largely preserved after forming the heterostructures, suggesting that the interlayer interaction is dominated by weak vdW coupling rather than strong covalent hybridisation.

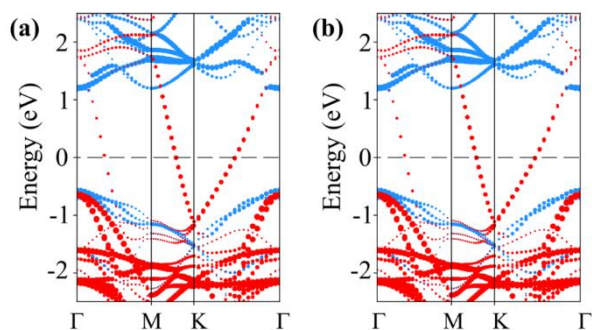


Fig. 4. Projected band structures of (a) Goldene/SMoSe and (b) Goldene/SeMoS heterostructures

Notably, the metallic nature of the Goldene monolayer is well maintained, with its bands crossing the Fermi level, while the semiconducting band gap of the Janus MoSSe layer remains nearly unchanged. The coexistence of metallic and semiconducting states near the interface leads to the formation of metal-semiconductor contacts in both the Goldene/SMoSe and Goldene/SeMoS heterostructures. Such contacts are essential for charge injection and transport in nanoelectronic devices and highlight the potential of Goldene as an effective two-dimensional metal electrode.

Furthermore, the relative alignment between the Fermi level of Goldene and the band edges of the MoSSe layer gives rise to Schottky-type contacts in both heterostructures. For both the Goldene/SMoSe and Goldene/SeMoS heterostructures, the Fermi level is located closer to the valence band maximum (VBM) of the MoSSe

layer, resulting in a *p*-type Schottky contact. The Schottky barrier height at the metal-semiconductor interface can be evaluated from the relative position of the Fermi level of the metal and the band edges of the semiconductor. Specifically, the *n*-type and *p*-type Schottky barrier heights are defined as $\Phi_{B,n} = E_{CBM} - E_F$ and $\Phi_{B,p} = E_F - E_{VBM}$, where E_{CBM} and E_{VBM} denote the energy of the CBM and VBM of the semiconducting MoSSe layer, respectively. E_F is the Fermi level of the heterostructure. The calculated *n*-type (*p*-type) Schottky barriers for the Goldene/SMoSe and Goldene/SeMoS heterostructures are 1.20 (0.57) eV and 1.01 (0.67) eV, respectively. This indicates that both heterostructures form *p*-type Schottky contacts because the *p*-type barriers are significantly smaller than the corresponding *n*-type ones. As depicted in Fig. 4, for both the Goldene/SMoSe and Goldene/SeMoS heterostructures, the Fermi level is located closer to the VBM of the MoSSe layer, confirming the formation of a *p*-type Schottky contact. This *p*-type Schottky behaviour highlights the potential of Goldene as an effective hole-injecting electrode for Janus MoSSe-based heterostructures.

To further elucidate the interfacial electronic interaction and charge redistribution in the Goldene/SMoSe and Goldene/SeMoS heterostructures, we calculate and analyse the charge density difference, as shown in Fig. 5. The charge density difference is defined as $\Delta\rho = \rho_{\text{Goldene/MoSSe}} - \rho_{\text{Goldene}} - \rho_{\text{MoSSe}}$, where $\rho_{\text{Goldene/MoSSe}}$, ρ_{Goldene} , and ρ_{MoSSe} represent the charge densities of the heterostructure, isolated Goldene, and isolated Janus MoSSe monolayers, respectively. One can find that electron depletion is mainly observed in the Goldene layer, confirming that Goldene acts as an electron donor upon heterostructure formation. In addition, a pronounced interfacial charge rearrangement is observed, revealing electron transfer between the two constituent layers. This behaviour can be attributed to the pillow (push-

back) effect induced by Pauli repulsion at the interface, which drives electrons away from the contact region and leads to the formation of an interfacial dipole. This interfacial charge transfer

shifts the Fermi level closer to the VBM of the MoSSe layer, confirming the formation of a *p*-type Schottky contact at the Goldene/MoSSe interface.

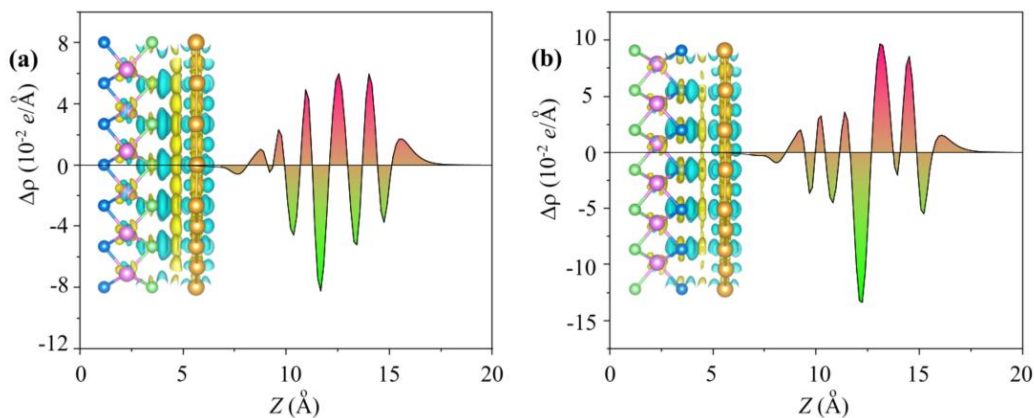


Fig. 5. Planar-averaged charge density difference of (a) Goldene/SMoSe and (b) Goldene/SeMoS heterostructures along out-of-plane direction. The insets show the corresponding charge density difference isosurfaces, where the yellow and cyan regions represent electron accumulation and electron depletion, respectively.

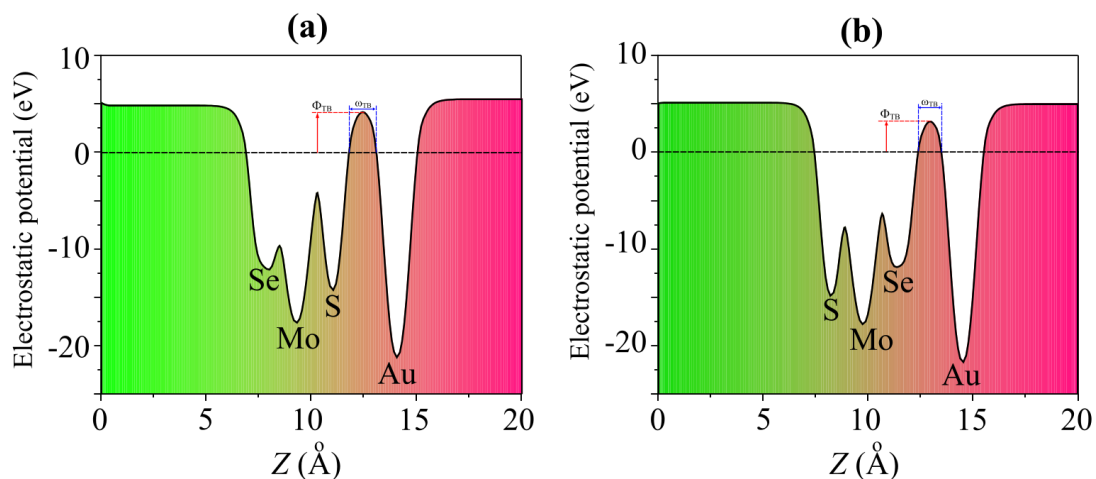


Fig. 6. Planar-averaged electrostatic potentials of (a) Goldene/SMoSe and (b) Goldene/SeMoS heterostructures along out-of-plane *z* direction

The planar-averaged electrostatic potentials along the out-of-plane direction for the Goldene/SMoSe and Goldene/SeMoS heterostructures are illustrated in Fig. 6. It can be seen that the electrostatic potential of the Goldene layer is consistently deeper than that of the MoSSe layer for both stacking configurations. This potential difference indicates that Goldene possesses a lower electrostatic potential compared with the Janus MoSSe monolayer. As a

consequence, electrons spontaneously transfer from Goldene to the MoSSe layer upon contact in order to reach electrostatic equilibrium. This electron transfer leads to the formation of an interfacial dipole and a built-in electric field pointing from the Goldene layer toward the MoSSe layer. The resulting internal electric field shifts the band edges of the MoSSe layer relative to the Fermi level, driving the Fermi level closer to the valence band maximum. As a result, *p*-type Schottky

contacts are formed in both the Goldene/SMoSe and Goldene/SeMoS heterostructures.

Furthermore, the tunnelling probability of the Goldene/MoSSe heterostructures is evaluated by using the following equation

$$T_p = \exp\left(-\frac{4 \times \pi \times \omega_{TB} \times \sqrt{2 \times m_e \times \Phi_{TB}}}{\hbar}\right)$$

where ω_{TB} and Φ_{TB} denote the tunnelling width and height of the Goldene/MoSSe heterostructure, as illustrated in the insets of Fig. 6. Our calculations reveal that the obtained ω_{TB} and Φ_{TB} values for the Goldene/SMoSe heterostructure are 1.41 Å and 4.40 eV, respectively, resulting in the tunnelling probability of 5.04 %. In contrast, the corresponding ω_{TB} and Φ_{TB} values for the Goldene/SeMoS heterostructure are 1.28 Å and 3.93 eV, respectively, yielding a tunnelling probability of 7.71 %. These values of the heterostructures are comparable with those obtained in other vdW heterostructures [22, 23].

4 Conclusion

In this paper, we computationally designed a novel metal-semiconductor Goldene/Janus MoSSe heterostructure and systematically investigated its electronic properties, contact characteristics, and interfacial charge transfer. The results demonstrate that the Goldene/Janus MoSSe heterostructure is energetically favourable and thermodynamically stable. At equilibrium, the heterostructure is predominantly governed by weak van der Waals interactions, which preserve the intrinsic electronic properties of the constituent monolayers and facilitate experimental fabrication. Furthermore, the Goldene/Janus MoSSe heterostructure forms a *p*-type Schottky contact, with Schottky barrier heights of 0.57 and 0.67 eV for the Goldene/SMoSe and Goldene/SeMoS stacking configurations, respectively. Charge density difference analysis further reveals that electrons are transferred from the Goldene layer to the MoSSe layer in both

stacking configurations, confirming the electron-donating role of Goldene and contributing to the built-in electric field at the interface. These findings highlight the potential of Goldene as an effective two-dimensional metal electrode for Janus MoSSe-based nanoelectronic devices.

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