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Electronic structure due to hydrogen and vanadium as substitutional impurities in InP

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The self-consistent local-density theory is used in a cluster model to calculate the charge distribution, one-electron energy spectra, and the density of states for pure InP and for H and V substituted at the In site. The pure semiconductor gap is found to be 0.8 eV, consistent with experiments. The hydrogen impurity introduces a trapping center at $E_v+0.37$ eV in the gap region—a semi-insulating-like behavior. The transition metals are generally found to introduce deep levels in the gap region, but for vanadium we find the gap swept clean of any impurity level, with the last partially occupied state close to the bottom of the conduction band. This is consistent with deep-level transient spectroscopy experiments where no vanadium-related deep levels in the band gap are found down to 4 K.

I. INTRODUCTION

Semiconductors with different impurities as dopants are of much interest in the production of efficient technological devices like solar cells, microwave devices, and optoelectronic elements. Among the III-V semiconductors that have attracted much attention are GaAs, GaP, and InP. InP has the higher mobility and is thus a potential candidate for high-speed switching devices. It has a promising technological future, providing preparation and purification problems can be overcome.

Impurities can change the Fermi energy with the introduction of energy levels in the gap region. These impurity levels act as trapping centers which control the electronic properties. It is known that proper positioning of hydrogen atoms can clean the gap of any impurity level in silicon[1] or germanium[2] and removes the *EL*2 impurity level in GaAs.[3] Few experimental data of a similar nature exist for InP. It is known that the alkali metals with a single *s* electron do not passivate the dangling bonds in InP. Li and Na produce levels close to the band edges, called shallow levels, whereas the introduction of K results in a level close to the midgap region, called a deep level.[4] In the same series, H, with its single 1*s* electron, is an interesting dopant to study theoretically.

Chromium doping is known to make GaAs semi-insulating. Iron in InP behaves in a similar manner; the resistivity of Fe-doped InP is an order of magnitude greater than that of Co-doped InP.[5] Recently, the electronic properties of different transition metals (Cr through Cu) as impurities in InP have been studied theoretically by Khowash *et al.*[6] using a multiple-scattering cluster approach. The transition metals were found to introduce deep levels (i.e., levels far from the conduction- or valence-band edges) whose valency is not clearly understood. On experimental grounds[7] vanadium was expected to create a deep level near the middle of the band gap. The experimental results seem to be crystal growth dependent,[8-10] so that V may be considered a controversial dopant in III-V semiconductors. Various experiments such as electron paramagnetic resonance (EPR), photocapacitance, Zeeman spectroscopy, and deep-level transient spectroscopy (DLTS) are able to resolve the degeneracy and symmetry of the electronic states, deep levels, structure of metal-semiconductor interfaces, etc. In order to provide first-principles theoretical models for comparison with forthcoming experimental data, we have undertaken calculations to clarify the electronic structure associated with selected substitutional impurities.

II. THEORETICAL METHOD

A. Self-consistent embedding

We obtain approximate solutions of the Hartree-Fock-Slater equations using a discrete-variational method[11-14] (DV-$X\alpha$), with basis functions describing a cluster scooped out of the solid. The rest of the solid is taken into account by generating a microcrystal surrounding the cluster. In other cluster approaches like the multiple-scattering $X\alpha$ (MS-$X\alpha$) method, hydrogen atoms are often placed in the last shell of atoms within the charged Watson boundary sphere to saturate the surface dangling bonds in semiconductors. Sometimes better results may be obtained by relaxing the hydrogen-ligand bond length by a few percent. Proper charges are then put on the Watson sphere to neutralize the cluster. In the present model, however, we generate a microcrystal consisting of 250–300 atoms to simulate the rest of the solid. The total charge density is then written as

$$\rho_{\rm tot}(\mathbf{r})=\rho_{\rm cluster}(\mathbf{r})+\rho_{\rm crystal}(\mathbf{r}) .$$

Each atom in the microcrystal contributes a spherically symmetrized Coulomb potential and contributes to the exchange interaction. The sum of these potentials is the resultant nonspherical cluster potential. The cluster eigenfunctions are then expanded as a linear combination of atomic orbitals (LCAO), here taken as numerical atomic or ionic solutions. The atomic potential binds

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only a limited number of states. To generate additional unoccupied states and expand the variational freedom of the basis, a potential well of 2 a.u. extending out to a radius of 6 a.u. is introduced for each atomic type. The ground-state electronic configurations of P and In can be written as [Ne] $3s^2 3p^3$ and [Pd] $5s^2 5p^1$, where [Pd] means that the orbitals 1*s* through 4*d* are treated as frozen core. Orbitals 1*s*, 2*s*, and 2*p* for H, 3*s* and 3*p* for P, 3*d* and 4*s* for V, and 5*s* and 5*p* for In are considered in the valence expansion. The Rayleigh-Ritz variational procedure determines the expansion coefficients and approximate eigenvalues. A discrete set of sampling points in the configuration space is choosen. The familiar matrix Schrödinger equation $H\psi = ES\psi$ is then solved self-consistently with the matrix elements defined as weighted sums over a set of sample points $\mathbf{r}_k$,

$$H_{ij} = \sum_k W(\mathbf{r}_k)\Phi_i^*(\mathbf{r}_k)H\Phi_j(\mathbf{r}_k) , \quad (1)$$

$$S_{ij} = \sum_k W(\mathbf{r}_k)\Phi_i^*(\mathbf{r}_k)\Phi_j(\mathbf{r}_k) , \quad (2)$$

to obtain energy eigenvalues and eigenfunctions. Here, Φ_i denotes the basis functions chosen as a linear combination of atomic orbitals. The details of the method are discussed elsewhere.[11-14]

B. Interpretation of excitation spectra

It is well known that local-density (LD) theory, with exchange-correlation potentials based upon a uniform gas model, is unable to reproduce the gap accurately in ground-state calculations. The ground-state energy differences differ from those found from ground to excited-state transitions mainly due to the neglect of self-interaction effects. The two results, however, may be similar when the change in potential is small. The self-interaction corrections can be accounted for approximately in a localized state when a transition-state calculation is performed by removing half an electron from the initial (filled) level to the final (unoccupied) state. The band-structure calculations of Bachelet and Christensen[15] (linearized muffin-tin orbitals) and Min and Freeman[16] (linearized augmented plane-wave method) using the local-density theory find a gap of 0.25 eV for GaAs which is characteristically much less than the experimental value of 1.5 eV. MS-$X\alpha$ cluster calculations by Fazzio *et al.*[17] predict a band gap of 1.17 eV for GaAs. Cluster LD calculations for other group-IV and -III-V semiconductors also predict fairly good band gaps,[18-22] for reasons which probably are due to the semilocalized exchange hole arising from cluster-localized wave functions.

Since the proton is light, thermal and zero point motion about a trapping site may be considerable. If the minimum of the proton potential is off the In nuclear site, we may expect to find symmetry-induced splittings in the electronic spectra. In the absence of experimental data we have chosen to consider the simplest high-symmetry substitution geometry. Total energy calculations to explore the possibility of displacement and local lattice distortion could be very interesting, but are beyond the scope of the present work. Tight-binding calculations on hydrogen in amorphous Si by Robertson[23] suggest that rearrangement of neighboring atoms can displace defect levels by approximately 0.5 eV.

III. RESULTS AND DISCUSSION

We used the embedded cluster method described above to calculate the volume charges, Mulliken populations, one-electron energies, and the density of states for pure InP and for substitutional hydrogen and vanadium impurities in InP at the In site (see Table I). For the "perfect" cluster, we have taken an indium atom at the center of a tetrahedron formed by four phosphorus at the nearest-neighbor sites and 12 indium at the next-nearest-neighbor shell (InP_4In_{12}). The "defect" clusters are formed by replacing the central indium with the desired impurity (HP_4In_{12} and VP_4In_{12}).

A. Electronic structure of the host

Only valence electrons are considered in our discussion, as they are of importance in electrical conductivity and optical processes. For the pure InP, the calculated central cation and anion ionicities (Table I) are nearly equal (0.35), differing slightly due to the non-stoichiometric nature and size effects of the 17-atom cluster.

The self-consistent one-electron spectra of the three clusters considered are presented in Fig. 1. The energy levels are designated according to the irreducible representations of the tetrahedral point group. For pure InP, the last filled level is of t_2 symmetry and the first empty level is of a_1 symmetry, as is also seen in previous band-

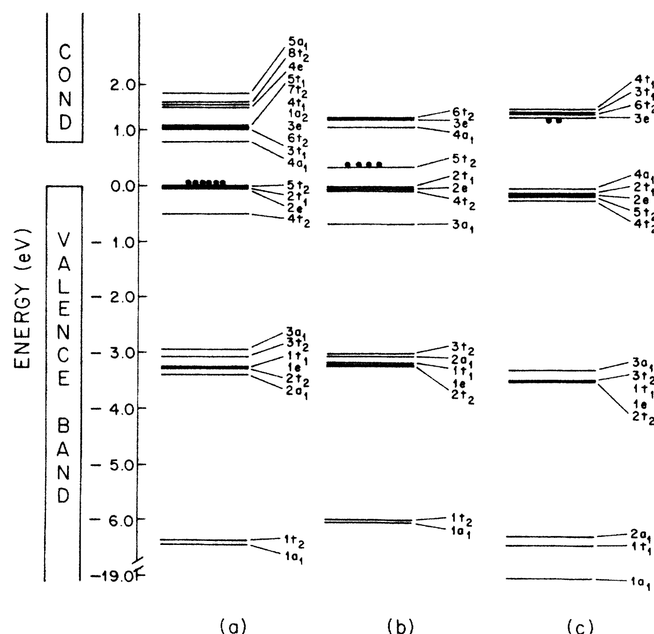

FIG. 1. Self-consistent one-electron energy spectrum of (a) InP, (b) InP:H, and (c) InP:V.

TABLE I. Volume charges and the Mulliken population analysis for InP, H, and V as impurities in InP, at the In site.

	Net volume charge (integration over atomic Wigner-Seitz cell)				
	InP		H:InP		V:InP
In	0.35		0.26		0.28
P	−0.36		0.02		−0.84
Impurity			−0.17		3.05
			Mulliken population analysis		
	InP		H:InP		V:InP
In 5s	1.96		1.93		1.90
5p	0.71		0.81		0.82
Net charge	0.33		0.26		0.28
P 3s	1.96		1.96		1.95
3p	3.38		3.03		3.85
Net charge	−0.35		0.01		−0.80
		H 1s	0.75	V 3d	0.01
		2s	0.29	4s	1.98
		2p	0.10		
Net charge			−0.14		3.01

structure and cluster calculations[19,20,24–26] on similar compounds. These levels form the valence-band and the conduction-band edges, respectively. The difference in energy between the two band edges, i.e., the band gap, is calculated to be 0.8 eV, using the ground-state potential. A transition-state calculation enhances the band gap by 0.1 eV. This can be compared with the experimental value of 1.34 eV.[27]

Isolated cluster calculations were also performed without embedding for pure InP with hydrogen in the second-nearest-neighbor position (InP_4H_{12}) as dangling-bond saturators at the surface. The band gap in this case is found to be reduced to 0.46 eV. At this stage, one can vary the position of the second nearest neighbors or their nuclear charge to improve the band gap and/or move hydrogenic states out of the gap region. The band gap increased by 0.06 eV on reducing the hydrogen nuclear charge by 0.2*e*. Since the embedding scheme leads to a gap of 0.8 eV, our calculations suggest the embedding leads to a better approximation to the local environment, without introducing the troublesome and spurious levels due to hydrogenic termination.

B. Electronic structure of InP:H

When hydrogen is placed at the In site, both the surrounding indium and phosphorus tend to be more atomiclike as compared to the charge distribution in the host: i.e., the ionic charge is reduced (Table I). From the Mulliken population analysis, we find charge transferred to H; it is an acceptor with 0.14*e* excess, and the neighboring P is essentially neutral. The reduction in charge on P in turn leads to a reduced ionicity (0.26) on the second-neighbor In sites. Although the electronegativities of P and H are equal ($\chi_H=2.1$, $\chi_{In}=1.5$, and $\chi_P=2.1$),[28] we see that the impurity modifies the charge distribution considerably.

For hydrogen as impurity, a t_2 level moves into the band gap. This level, due to broken In—P bonds, is usually termed as a dangling-bond hybrid. Other semiconductor calculations[23–26] on materials such as Si, GaAs, and InP also predict levels of this kind in the gap region. The t_2 level, composed of 3% H, 42% In, and 55% P, contains four electrons and is placed at 0.37 eV above the valence-band edge. Earlier MS-$X\alpha$ calculations by Khowash *et al.*[6] predicted a level exactly in the midgap region for iron as a substitutional impurity at the In site. Iron is known to be a useful dopant for making semi-insulating substrates of InP for technological use. Again, potassium, with a single *s* electron, is calculated[4] to introduce a deep level and behave like a semi-insulator. With a trapping center close to the midgap region hydrogen is also likely to behave in a similar manner.

C. Electronic structure of InP:V

We consider the situation in the analogous GaAs compound first, to form the basis for some comparisons. Vanadium was doped in GaAs as an alternative to semi-insulating GaAs:Cr, which has a large Cr diffusion coefficient.[26] The published results seem to be contradictory: Hall-effect and resistivity[27] experiments predict vanadium to act as a donor, in contrast to similar experiments[28] for a liquid-encapsulated Czochralski (LEC)-grown crystal where it is a midgap acceptor. DLTS experiments[29] find no electrically important gap levels in GaAs. On the other hand, in GaP, the proposed energy level scheme from optical transitions and the photoconductivity[30] spectrum identifies vanadium as a deep acceptor with additional levels close to the conduction-band edge that may merge into the conduction band if the pressure or temperature is varied. The impurity, therefore, is a strong compensator of the original *n*-type material with a high resistivity. Despite this, the optical

spectroscopic study of Kaufmann *et al.*[31] finds that GaP:V continues to remain *n*-type as the concentration of vanadium is increased. The optical properties like luminescence and absorption spectra associated with vanadium doping are also reported[31] to vary little in the III-V compound. Thus vanadium seems to be a poorly characterized dopant in the III-V semiconductors and a detailed study is necessary for a better understanding.

Luminescence spectra in InP:V were observed to be similar to that of GaAs:V;[7,32] no vanadium-related levels were detected in the gap. From Zeeman spectroscopy measurements Skolnick *et al.*[33] identified the vanadium center to be trivalent, whereas Lambert *et al.*[7] interpret their luminescence spectra in terms of V^{2+}. Recent Zeeman[34] and EPR (Ref. 35) measurements confirm vanadium to be trivalent and assert the absence of any vanadium-related levels in the gap.

We tabulate (Table I) the charge distribution for vanadium (ground-state basis: [Ar] $3d^3 4s^2$) as a substitutional impurity at the In site. From Mulliken population analysis we find vanadium to be trivalent, in the $3d^{0.01}4s^{1.98}$ configuration. Spin-unrestricted calculations in the embedded scheme were also performed and the net spin on the vanadium site was found to be less than or equal to $0.01\mu_B$, with the $3d$ electrons completely depopulated in the process of charge redistribution. Such high ionic configurations are reported in Cr-doped GaP,[36,37] GaAs,[38,39] and InP.[37] This can also be compared with the formal oxidation states of 4+ and 5+ of V in gas-phase tetrahedrally coordinated molecules like VCl_4 (Ref. 40) and the vanadate[41] ions $(VO_4)^{3-}$. A similar behavior in vanadium-doped GaAs is observed, where the electron-spin-resonance spectrum of semi-insulating GaAs:V contains a characteristic signal which is identified as V^{3+}. In contrast the host In ion in the second-nearest-neighbor position is found to be nearly neutral with $5s^{1.94}5p^{0.84}$ configuration. More charge is transferred from vanadium to phosphorus as compared to indium. This is consistent with the Pauli electronegativity scale ($\chi_V = 1.7$, $\chi_P = 2.1$, and $\chi_{In} = 1.5$).

We find that the partially filled $3e$ level, of mostly In $5p$ character, is pushed inside the conduction band of the pure semiconductor. The band gap is swept clean of impurity levels and the last occupied level in the ground state is close to the bottom of the conduction band, in contrast to the deep levels introduced by other transition-metal dopants.[6] In our theoretical calculations we thus find the gap contains no impurity levels. The calculated Fermi level is at 0.002 eV below the partially filled $3e$ level as compared to the experimental Hall-effect[32] value of 0.004 eV. Our results are also consistent with the deep-level transient thermal spectroscopy experiments[7] where no vanadium-related levels are revealed in the gap even at 4 K.

D. Density of states

The DV-LCAO self-consistent cluster energy levels obtained in the embedded scheme are broadened by a Lorentzian of fixed width to simulate a continuous density of states (DOS). Figure 2 shows the total density of states for the pure InP semiconductor. The P $3s$ levels lie at the bottom of the valence band [Fig. 3(a)], centered at -7.5 eV. The In $5s$ peak [Fig. 3(c)] is about 3.7 eV above the P $3s$ peak. The $3p$ functions of phosphorus hybridize with the $5p$ and $5s$ functions of In just below the valence-band edge. The contribution of the P $3p$ reduces from 61% to 4% as we go across the valence-band edge into the conduction-band edge. The $4a_1$ first unoccupied level is essentially s-like (see Fig. 1).

E. DOS of H impurity

For the hydrogen as impurity, the deep-lying P $3s$ and In $5s$ peaks show similar structure [Fig. 4(a)] to the undoped material but with a reduced energy separation of 2.8 eV. The In $5s$ peak moves towards the band edge, which is consistent with the charge transfer (see Table I). Close to the valence-band edge, the H $1s$ and $2s$ contributions are 37% and 14%, respectively. The $1s$ hydrogen bonding level [Fig. 4(b)] shows up at 0.8 eV below the valence-band edge. Figure 4(c) shows that the hydrogen $2s$ density of states peaks at 9.9 eV far up in the

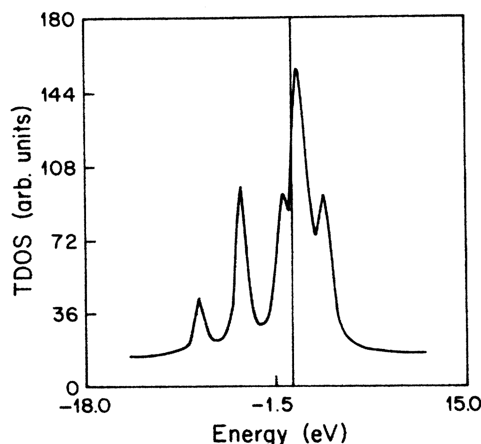

FIG. 2. Total density of states (TDOS) of host semiconductor InP.

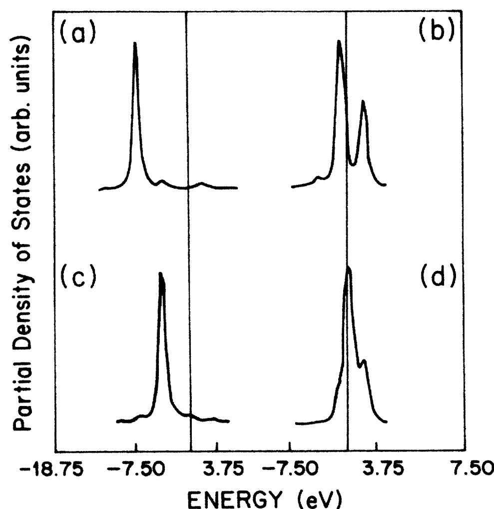

FIG. 3. Partial density of states (a) In $5s$, (b) In $5p$, (c) P $3s$, and (d) P $3p$.

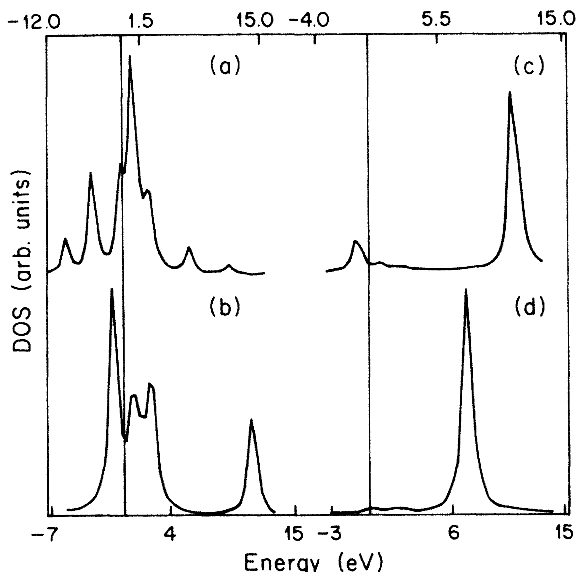

FIG. 4. (a) Total density of states of InP:H; (b) partial density of states of H 1*s* in InP:H; (c) partial density of states of H 2*s* in InP:H; and (d) partial density of states of H 2*p* in InP:H.

conduction band. However, there are weak components in the VB region contributing to bonding, and a "band tail" extending through the low-lying conduction-band states. The H 2*p* peak [Fig. 4(d)] is 4.1 eV below the H 2*s* peak. These 2*s*,2*p* excited-state contributions give some indication of the distortion and expansion of the hydrogenic wave function in the dielectric host medium. In principle, the excited states indicated in Figs. 4(c) and 4(d) can be probed by spectroscopic methods.

F. DOS of V impurity

Figure 5(a) shows the total density of states for the case of vanadium as an impurity at the indium site. The V 4*s* contribution [Fig. 5(b)] to the density of states is located at the bottom ($1a_1$) of the valence band. The filled $4a_1$ level now forms the upper valence-band edge. The doubly occupied In 5*p* level appears as the 3*e* state at the bottom of the InP conduction band. The P 2*s* and the In 5*s* separation is now 3.6 eV, being practically unaffected by vanadium doping. This could be due to the fact that when the central In is removed, three valence electrons are removed, and dangling bands are formed. With the introduction of vanadium, three 3*d* valence electrons are donated to rebuild the broken bonds.

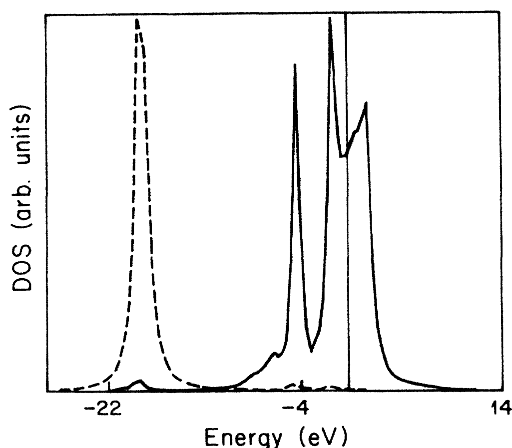

FIG. 5. (a) Total density of states of InP:V; (b) partial density of states of V 4*s* (dashed line) in InP:V.

IV. CONCLUSION

A self-consistent, local-density, discrete-variational, linear combination of atomic orbitals method has been used to calculate the charge distribution, the one-electron energy spectra, and the density of states of the pure InP semiconductor and for hydrogen and vanadium as substitutional impurities at the In site. The pure semiconductor gap of 0.8 eV is in fair agreement with the experimental value of 1.35 eV.

For a hydrogen impurity at the In site, a defect level of t_2 symmetry appears at 0.37 eV above the valence-band edge. Impurity levels in InP:Fe and InP:K are also reported to be in the midgap region, thus making the material semi-insulating. InP:H, with a trapping center close to the midgap region, is likely to behave in a similar manner.

When vanadium is introduced, no deep level is observed, in contrast to what is seen with other transition metals as dopants. The band gap is swept clean of impurity levels, consistent with the DLTS thermal spectroscopy experiments at low temperatures. Also, in the process of reaching self-consistency, vanadium becomes trivalent consistent with the recent EPR experiments. A spin-unrestricted calculation was also performed and the net spin on the vanadium site was found to be approximately 0, indicating a diamagnetic state, since the 3*d* electrons are completely depopulated in the process of redistribution. We find the Fermi level in InP:V to be at ≤ 0.01 eV below the conduction-band edge, which is in reasonably good agreement with Hall-effect results.

We have considered electronic properties of the pure semiconductor, and the idealized monatomic substitution on the In site. Actual crystals are contaminated with impurities like C, N, O, Si, etc. Apart from these, there can be vacancies, antisite defects, and other complex defects which can alter the electronic structure remarkably, due to the distortion in the symmetry structure and local bonding in the lattice. Neither lattice relaxation nor charge-compensating defects were considered in the present calculations. Further analysis of impurity states in InP and other III-V compounds which seeks to determine minimum energy configurations would be very useful.

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