# P a E G S a InA /InSb Q a D

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Using atomistic pseudopotential and configuration-interaction many-body calculations, we predict an excitonic ground state in the InAs/InSb quantum-dot system. For large dots, the conduction band minimum of the InAs dot lies below the valence band maximum of the InSb matrix. Due to quantum confinement, at a critical size calculated here for various shapes, the gap $E_g$ between InAs conduction states and InSb valence states vanishes. Strong electron-hole correlation effects are induced by the spatial proximity of the electron and hole wave functions, and by the lack of strong (exciton unbinding) screening, afforded by the existence of discrete 0D confined energy levels. These correlation effects overcome $E_g$, leading to the formation of a biexcitonic ground state (two electrons in InAs and two holes in InSb) being energetically more favorable (by $\sim$15 meV) than the dot without excitons.

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The formation of excitons in semiconductors and insulators usually requires energy, e.g., photons, for one has to excite carriers across the single-particle band gap $E_g$. There is a special interest, however, in the possibility of forming excitons exothermically, i.e., an "excitonic ground state" as envisioned by Mott [1] and Keldysh . [2]. Indeed, the electron-hole system exhibits a rich range of phases [3,4] as a function of the carrier density and effective-mass ratio $m_e/m_h$, including various excitonic insulating states such as molecular solid, exciton liquid, Mott insulator, and also various metallic phases. The excitonic ground state is of fundamental interest in itself because excitons can be a better alternative to atoms for studying Bose-Einstein condensation [5,6] on account of the lighter excitonic mass, thus higher condensation temperature. It is natural to search for excitonic ground states in systems where $E_g$ is small, yet the screening is weak enough so as to prevent unbinding of the exciton. The search in [7] has thus focused on gap semiconductors and semimetals to reduce screening, but excitonic ground states have not been conclusively observed so far in such systems. Ground state excitons were also searched in , specifically in spatially indirect quantum wells [8,9], where electrons and holes are confined in different spatial regions. In "type II" systems such as GaInAs/InP or CdTe/CdSe, electrons are localized in the well, whereas holes are localized on the barrier, so screening is weak, but $E_g$ is finite. In contrast, in "type III" heterostructures such as [10] InAs/GaSb, the conduction band minium (CBM) of the InAs well is lower than the valence band maximum (VBM) of the GaSb barrier, so at certain well thickness one can have $E_g \rightarrow 0$ [10], as well as separation of electrons from holes. Thus, at this thickness, one could expect an excitonic ground state if the electron-hole correlation energy will be large enough to stabilize the complex. Recent experiments [11] show evidence for an existing excitonic ground state in type III InAs/$\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{Sb}$ quantum-well superlattices; however, the binding energy was small (estimated at $\sim$3–4 meV) and strong magnetic fields are needed to stabilize the system. This is because in a 2D periodic well or superlattice, extended states exist in the in-pane direction leading to rather weak excitonic binding.

The advantage of a type III system can, however, be utilized without the disadvantage of 2D periodicity underlying a quantum well, if one considers a type III *0D* (QD). The well known InAs/$\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{Sb}$ epitaxial system [11] is inappropriate here, since it is lattice matched, so dots will not form in a strain-induced Stranski-Krastanov (SK) growth [12]. We propose here a new dot/matrix system, InAs/InSb, which has a type III band alignment [13], and a lattice mismatch, and is hence amenable to epitaxial SK growth. Using an empirical pseudopotential approach [14], we find that as the dot size is reduced, electron levels localized on InAs move up in energy, whereas hole states, localized at the interface, initially above the electron levels, move down in energy. The system reaches a degeneracy $E_g \sim 0$ of electron and hole single-particle levels at a critical size, predicted here for different dot shapes. As a result of the 0D confinement of both electrons and holes, there is but a small number of fully discrete bound states, so screening is limited, helping the binding of the particles. Furthermore, the strain in the lens-shaped or spherical dots localized the holes at the interface near the dot, thus offering proximity which is conducive to electron-hole binding. Using many-body configuration interaction (CI), we find that consequently, at the critical size, the exciton is bound by as much as $\sim$15 meV $\gg E_g$, thus forming an excitonic ground state. Our study characterizes theoretically the properties of the excitonic ground state in this system, offering experimentally testable predictions.

. The customary way of selecting a dot/matrix system [12] is to require that the dot material has a smaller gap than the matrix material (e.g., InAs/GaAs or CdSe/ZnSe) so that all car-

To see whether the shape of the dot affects these conclusions, we performed similar calculations for spherical InAs/InSb QDs. The critical diameter for the single-particle band gap closure is now around $2R = 64$ A. The calculated exciton and biexciton energies are shown in Fig. 4(b) for two diameters (52 and 64 A). For the $2R = 64$ A dot, we find an exciton energy of $E_{\mathrm{X}} = -22$ meV, and a biexciton energy of $E_{\mathrm{XX}} = -39$ meV. Again the two electron-hole-pair state is the ground state and we have $_{X} = 19$ meV and $_{XX} = -5$ meV. The biexciton is also unbound.

[illegible] The two electron-hole-pair ground state is similar to a helium atom in the sense that there are two positive and two negative Coulomb bound charges. These states can be identified as ‘‘excitonic molecule’’ states [4]. The calculated permanent electric dipole moment $\mathbf{p} = \int \rho( )d^3x$ for the exciton and biexciton of the lens-shaped dot D2 are aligned along [001] direction (growth direction), and amount to $p_z = 3.58e$ A for the exciton and $p_z = 7.16e$ A for the biexciton. These dipoles could be measured experimentally and since the exciton binding energy is so high ($_{X} \sim 15$ meV), it can be studied at rather high temperatures.

Recent developments in epitaxial growth made it now possible to grow arrays of QDs [23]. Given these excitonic dipoles, it is interesting to study the collective behavior of excitons in the QD arrays due to dipolar interactions. At a [illegible], where the QDs are far apart, the excitons behave like in the single dot and couple only weakly via dipole-dipole interactions. This is the classic problem of Bose-Einstein condensation (BEC) in dipolar Bose gases, which is currently attracting a lot of attention [24,25]. The BEC of dipolar gases may have various phases depending on details of the interactions [26]. Since excitons have lighter masses and stronger dipole-dipole interactions than atoms, they are therefore ideal candidates for the study of the different BEC phases. In the case of dot arrays, the exciton energy in a single dot $E_x < 0$ signals only the instability towards the excitonic insulator, where it must be renormalized by the dot-dot interactions. Furthermore, the size distribution and disorder of the QD lattice may lead to a more complicated ‘‘Bose glass’’ phase [27,28]. Thus, the excitonic ground states in dot arrays bring up challenging and interesting problems to both theorists and experimen-