Density-functional study of size-dependent properties of Cd_mSe_n clusters

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(Received 16 May 2003; revised manuscript received 13 August 2003; published 11 December 2003)

We present results of density-functional calculations of structural and electronic properties of naked, stoichiometric zinc-blende-, wurtzite-, and rocksalt-derived CdSe clusters as a function of size of the cluster and of nonstoichiometric CdSe clusters with zinc-blende-derived structure. We have optimized the structure whereby our initial structures were taken as spherical parts of the crystals. The calculations were performed by using a parametrized linear combination of atomic orbitals–density-functional theory–local-density approximation scheme. Our results include the radial distribution of atoms and of Mulliken populations, the electronic energy levels, the band gap, and the stability as a function of size and composition.

I. INTRODUCTION

Nanoparticles can be considered as intermediates between a solid and a molecule. Their fundamental properties depend critically on their size.[1–5] The size dependence arises from quantum-confinement effects, i.e., the reduction of the band structure into discrete quantum levels resulting from the limited size of the particles.[6–9] Thus, by varying the semiconductor material as well as the size of the nanoparticles, it is possible to tune electrical and optical properties, which makes these materials promising materials for a number of applications such as LED's (light emitting diodes) and nanosized switching devices.[2]

Chemical techniques for controlling nanocrystal size and the accompanying development of a physical picture of finite-size effects were pioneered in the early 1980s by Brus through his work on solution-phase synthesized II-VI quantum dots.[10] Since then, a steady series of advances in the chemical preparation of such nanocrystals has made II-VI nanocrystals the prototypes for the investigation of finite-size effects (see, e.g., Refs. 11–18). In particular, nanocrystals of CdSe are interesting, also because of a fascinating blinking, or on/off behavior, of the photoluminescence (see, e.g., Ref. 19). In order to understand this and many other phenomena, a detailed understanding of the electronic energy levels is of paramount importance, e.g., through complementary theoretical studies on well-defined systems. However, such studies are challenging because of the many structural degrees of freedom combined with a relatively low symmetry and the large size of the system. Therefore, most often such studies make more or less severe assumptions on the structure and/or apply less accurate computational methods. Moreover, effects of ligands are often approximated if included at all, and in most studies isolated particles in the gas phase are studied, whereas many experimental studies are carried through in solution.

In a previous work,[20] we have reported results of a systematic study of the electronic and structural properties of a whole series of large stoichiometric Cd_nS_n clusters. We considered structures that were obtained by relaxing spherical parts of both the zinc-blende and wurtzite crystal structure. That study was, to the best of our knowledge, the first one where structural properties of a series of also larger clusters were studied, and it has later been supplemented by a related study on stoichiometric and nonstoichiometric In_mP_n clusters[21] as well as stoichiometric clusters of CdSe and ZnO whose structures were derived from the wurtzite or the zinc-blende crystal structure.[22] In order to make the calculations possible we employed the simplified LCAO-DFT-LDA (linear combination of atomic orbitals–density-functional theory–local-density approximation) scheme.[23–25]

In this paper we present our LCAO-DFT-LDA results of the size-dependent structural and electronic properties of both stoichiometric and nonstoichiometric Cd_mSe_n clusters with $n+m$ up to ≈ 200. Moreover, since the structure of CdSe nanocrystals may change to the rocksalt structure upon application of pressure,[26,27] this structure was included in our study, too. Due to the large interest in nanocrystalline CdSe the present study is a natural and highly relevant extension of our earlier studies, and by comparing with those we will also be able to identify material-specific properties.

CdSe nanocrystals have been the focus of many previous theoretical studies. Some of the earliest studies employed the effective-mass method whereby the underlying structure of the cluster becomes of only secondary importance.[28,29] In later studies,[30–34] the optical properties (including excitonic excitation energies) have been studied using the empirical pseudopotential method so that the structure of the cluster is included but not relaxed. In some cases the dangling bonds on the surface have been passivated, and using this approach also large systems have been studied. Alternatively, various tight-binding methods that also take into account the positions of the nuclei have been applied.[35–42] Also in this case most studies have focused on optical properties, and the structure was not relaxed. An exception is the studies of Whaley and co-workers[39,40] where the changes of the electronic properties due to changes in the structure of the surface were studied although, however, without optimizing the structure. Finally, CdSe clusters have also been studied using parameter-free density-functional methods.[43–46] Troparevsky

and Chelikowsky[44] studied small naked stoichiometric Cd_nSe_n clusters ($n = 2-8$) and optimized the structure. On the other hand, Andersen *et al.*[45] studied slightly larger clusters but did not undertake any attempt of optimizing the structure. Most detailed are the studies of Ahlrichs and co-workers[43,46] who considered both ligand-capped clusters as well as naked ones. For the latter they optimized the structures completely up to $n = 7$ and subsequently considered (relaxed) parts of the wurtzite crystal structure with up to almost 200 atoms.

In the present work we have considered spherical parts of zinc-blende, wurtzite, and rocksalt crystals and subsequently let their structures relax to their closest total-energy minima whereby all atoms were allowed to move. By putting the center of the sphere on the midpoint of a Cd-Se bond, stoichiometric Cd_nSe_n clusters are obtained, whereas we obtain nonstoichiometric Cd_mSe_n clusters by placing the center at a Cd or a Se atom. We shall discuss the structural relaxations and how these influence the electronic properties as well as compare the zinc-blende-, wurtzite-, and rocksalt-derived clusters and also compare stoichiometric and nonstoichiometric clusters.

The paper is organized as follows. In Sec. II a brief outline of the computational method employed here is given and the results of the calculations are presented in Sec. III. In Sec. IV our findings are summarized.

II. THEORETICAL METHOD

We have employed the parametrized density-functional tight-binding method of Seifert and co-workers,[23–25] which has been described in detail elsewhere, and, therefore, here shall be only briefly outlined.

The approximate LCAO-DFT-LDA method is based on the density-functional theory of Hohenberg and Kohn in the formulation of Kohn and Sham.[47,48] The single-particle eigenfunctions $\psi_i(r)$ of the Kohn-Sham equations are expanded in a set of atomiclike basis functions ϕ_m with m being a compound index that describes the atom at which the function is centered as well as its angular and radial dependence. The functions ϕ_m are obtained from self-consistent density-functional calculations on the isolated atoms employing a large set of Slater-type basis functions.

The effective Kohn-Sham potential $V_{eff}(\vec{r})$ is approximated as a simple superposition of the potentials of the neutral atoms, $V_{eff}(\vec{r}) = \Sigma_j V_j^0(|\vec{r} - \vec{R}_j|)$. Furthermore, we make use of a tight-binding approximation, so that $\langle \phi_m | V_j^0 | \phi_n \rangle$ only is nonvanishing when ϕ_m and/or ϕ_n is centered at $\vec{R}_j$.

Then, the binding energy is approximated as the difference in the single-particle energies of the occupied orbitals of the compound and the isolated atoms, augmented with short-ranged pair potentials,

$$E_B \simeq \sum_i^{occ} \epsilon_i - \sum_m \sum_j^{occ} \epsilon_{jm} + \frac{1}{2} \sum_{j \neq j'} U_{jj'}(|\vec{R}_j - \vec{R}_{j'}|). \quad (1)$$

$U_{jj'}(|\vec{R}_j - \vec{R}_{j'}|)$ is determined from exact density-functional calculations on diatomics, i.e., in our study on the CdSe, Cd_2, and Se_2 molecules.
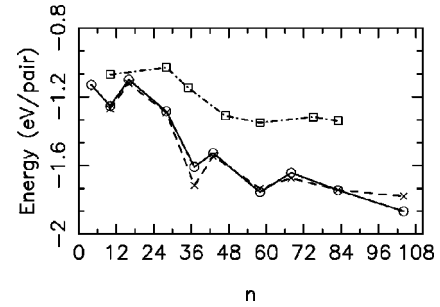

FIG. 1. Variation in the total energy per CdSe pair for stoichiometric Cd_nSe_n clusters as a function of n for (crosses) zinc-blende-, (circles) wurtzite-, and (squares) rocksalt-derived clusters.

Finally, only the $4d$ and $5s$ electrons of Cd and $4s$ and $4p$ electrons of Se were explicitly included in the calculations, whereas the other electrons were treated within a frozen-core approximation.

The present calculational scheme is constructed as being accurate for small (diatomic) molecules, whereas we attempt to use it for larger clusters. Therefore, to obtain an estimate of the accuracy of the method, we first performed calculations on infinite, periodic, crystalline structures. This led to optimized lattice constants for the zinc-blende structure of 5.96 Å, for the wurtzite structure of 4.26 and 6.96 Å, and for the rocksalt structure of 5.67 Å. The experimental values for the zinc-blende and wurtzite structures are (see, e.g., Ref. 49) 6.05, 4.30, and 7.01 Å, respectively. Thus, the structural parameters of the infinite crystalline material are well produced. The total-energy difference between the wurtzite and zinc-blende structures is found to be very small, i.e., 2 meV/atom with the zinc-blende structure being stabler. The small value is in accord with previous studies.[50,51] Although the theoretical studies find the zinc-blende structure to be stabler, in contrast to experimental findings, we consider the total-energy difference so small that a definite statement about the relative stability cannot be made. The rocksalt structure has a considerably higher energy (26 meV/atom higher than the wurtzite structure) again in agreement with earlier theoretical findings.[52] As a further test of the accuracy we also calculated the bulk moduli for the three crystal structures. We found 58, 60, and 64 GPa for zinc-blende, wurtzite, and rocksalt, respectively. The experimental value for wurtzite is 53.4 GPa (Ref. 53), i.e., in good agreement with our value.

III. RESULTS AND DISCUSSIONS

The first issue we shall address is the relative stability of stoichiometric Cd_nSe_n clusters. Due to the stoichiometry it is straightforward to compare the energy of different clusters.

In Fig. 1 we show the total energy per CdSe pair as a function of n for clusters derived from the three different crystal structures. As for the infinite crystal, the rocksalt structure is less stable than the two other structures, which also agrees with the experimental finding[26,27] that pressure is needed in order to obtain clusters with the rocksalt structure. The figure shows also that the relative stability of the zinc-blende and wurtzite clusters depends critically on n. The total-energy difference is significantly larger than the corre-
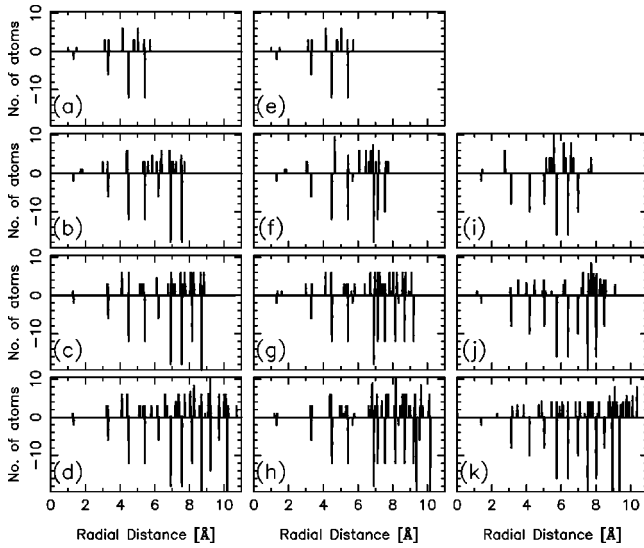
FIG. 2. Radial distribution of cadmium and selenium atoms for zinc-blende- (left column), wurtzite- (middle column), and rocksalt-derived clusters (right column) of different sizes: (a), (e) $Cd_{16}Se_{16}$; (i) $Cd_{35}Se_{35}$; (b), (f) $Cd_{37}Se_{37}$; (c), (g), (j) $Cd_{58}Se_{58}$; and (d), (h), (k) $Cd_{83}Se_{83}$. In each panel, the upper part is representing the relaxed and the lower part the unrelaxed structure, respectively. The radial distance is defined through Eq. (3), and the y axis gives the number of atoms with a certain radial distance.
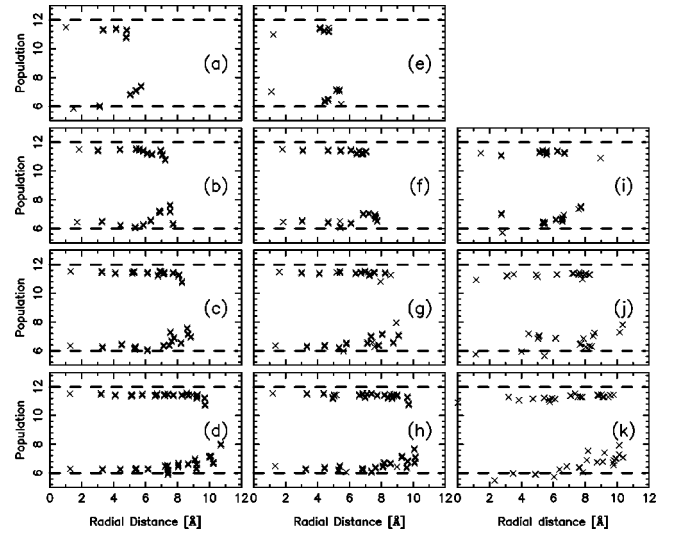

FIG. 3. Radial distribution of Mulliken gross populations for the valence electrons of Cd and Se atoms for the same structures as in Fig. 2, i.e., for zinc-blende- (left column), wurtzite- (middle column), and rocksalt-derived clusters (right column) of different sizes: (a), (e) $Cd_{16}Se_{16}$; (i) $Cd_{35}Se_{35}$; (b), (f) $Cd_{37}Se_{37}$; (c), (g), (j) $Cd_{58}Se_{58}$; and (d), (h), (k) $Cd_{83}Se_{83}$. The horizontal dashed lines mark the values for the neutral atoms, i.e., 6 for Cd and 12 for Se.

sponding value for the infinite systems. This finding was also observed for CdS and InP clusters (see Refs. 20–22) but it is interesting to note that the question which structure is stabler for a given n depends not only on n (i.e., is not only a question of geometry), but also on the material (i.e., the curves for CdSe, CdS, and InP are different). The fact that the structure can switch between wurtzite and zinc-blende depending on size has also been observed experimentally.[54] Finally, the overall shape of the total-energy curves is in accordance with simple expectations that it consists of two parts, i.e., a volume part and a surface part and, hence, is of the form $A + Bn^{-1/3}$.

In describing the properties of the clusters we will introduce a radial distance for each atom. Thus, for a given Cd_mSe_n cluster we define the center as

$$\vec{R}_0 = \frac{1}{n+m} \sum_{j=1}^{n+m} \vec{R}_j, \qquad (2)$$

where the summation goes over all atoms of the cluster. Subsequently, the radial distance for the jth atom is defined as

$$r_j = |\vec{R}_j - \vec{R}_0|. \qquad (3)$$

We shall depict the various properties as a function of the radial distance, including the number of atoms, the Mulliken gross populations, and the distribution of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) frontier orbitals.

The radial distribution of atoms is shown in Fig. 2 for selected zinc-blende-, wurtzite-, and rocksalt-derived clusters. The figure shows the radial distances for both cadmium

and selenium atoms of the optimized structure (upper half) and of the initial geometry (lower half). From the figure it is evident that for the optimized structures the largest changes compared with the initial structure occur in the outer region of the cluster, i.e., up to around 3 Å from the outermost atoms (although also relaxations also further away from the surface can be identified). In this region, some atoms move away from the center of the cluster, whereas other approach the center. Inspecting the radial distribution of the Cd and Se atoms separately (not shown) it is found that only selenium atoms move outward whereas the cadmium atoms move inward. This different behavior of chalcogen and metal atoms is also found in our earlier work on CdS and InP clusters[20,21] as well as by Leung and Whaley[40] in their more phenomenological study of the properties of CdSe clusters. Moreover, similar structural relaxations have been found for surfaces of crystalline CdSe both in theoretical[55] and experimental[56] studies. Finally, also Deglmann *et al.*[46] found in their density-functional study of larger wurtzite-derived clusters significant structural relaxations.

In our previous work on CdS and InP clusters[20,21] we found it useful to analyze the electronic distribution by plotting the Mulliken gross populations as a function of the radial distance. For the stoichiometric Cd_nSe_n clusters we show these in Fig. 3. From the figure it is clear that similar to our findings for CdS and InP clusters the gross populations are markedly different from the values of the neutral atoms only in the outer parts of the cluster. In this region, an increased electron transfer from Cd to Se takes place for most systems in a surface region of 2–3 Å thickness. All these results suggest that the stoichiometric CdSe clusters possess a surface region of about 2.5 Å thickness, largely independent of structure and size. We mention that a careful inspec-
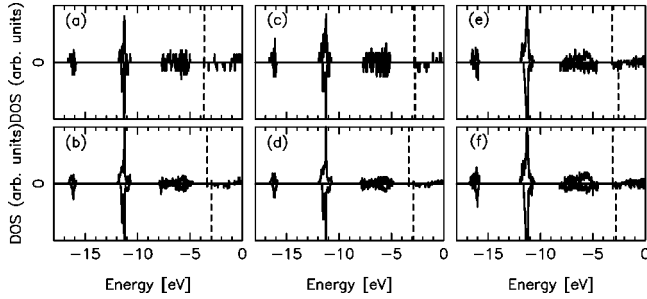
FIG. 4. Density of states (DOS) for different zinc-blende- (left column), wurtzite- (middle column), and rocksalt-derived (right column) clusters of different sizes: (a), (c) $Cd_{16}Se_{16}$; (e) $Cd_{58}Se_{58}$; and (b), (d), (f) $Cd_{83}Se_{83}$. The upper part of each panel is representing relaxed and the lower part unrelaxed structures, respectively. The vertical dashed lines mark the Fermi energy. Notice that the different panels have different scales on the y axis.
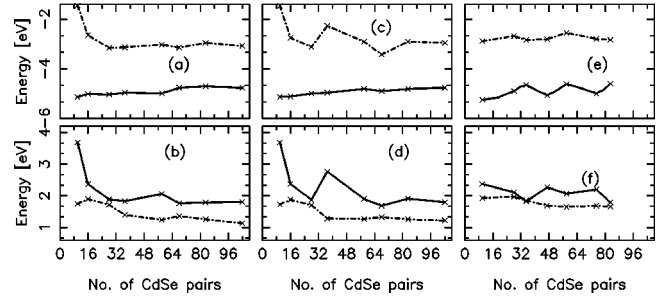

FIG. 5. Energy of (a), (c), (e) HOMO (lower curve) and LUMO (upper curve) as well as (b), (d), (f) HOMO-LUMO gap (solid curve) and relative total energy per CdSe pair (dashed curve) for stoichiometric zinc-blende- (left column), wurtzite- (middle column), and rocksalt-derived clusters (right column) as functions of the number of CdSe pairs.

tion of the figure shows that the outermost atoms are those with the smallest gross populations, i.e., Se atoms, as mentioned above.

In Fig. 4 we show the density of states, obtained by broadening the individual electronic levels slightly with Gaussians, for six representative systems of increasing size for clusters of wurtzite-, zinc-blende-, and rocksalt-derived structures. It is observed that the states below the Fermi energy arrange into separate bands. The band corresponding to selenium $4s$ functions lies in the range between -17 and -15 eV, the one corresponding to Cd $4d$ in the range -13 to -11 eV and, finally, the uppermost occupied band between -9 and -5 eV is formed mainly by Se $4p$ and partly by Cd $5s$ functions. Apart from the fact that for the larger clusters the bands are slightly broader, the other features are remarkably similar for all systems. Our results are in qualitative agreement with earlier theoretical studies on infinite[31,33,49,55,57,58] and finite[30,35–37,46] CdSe systems. E.g., Deglmann et al.[46] find in their density-functional calculations on wurtzite-derived Cd_nSe_n clusters with $n=30$, 44, and 99 Se $4s$ orbitals between -15 and -19 eV, Cd $4d$ orbitals between -11 and -15 eV, and Se $4p$ orbitals between -5 and -11 eV.

One of the surprising results of Fig. 1 is that the total energy is not a smooth function of size but shows strong size-dependent oscillations. We have shown[22] that this is a general finding for many naked stoichiometric AB semiconductor clusters and argued that this could be related to the so-called HSAB (hard acids and soft bases) principle of Pearson,[59] i.e., large-gap clusters are particularly stable. In Fig. 5 we show the energies of the HOMO and LUMO frontier orbitals as well as the energy gap between them together with the variation in the total energy. It is immediately seen that, as for CdS (Ref. 20) and InP (Ref. 21), the band-gap oscillates strongly as a function of size of the cluster, but also that the above-mentioned correlation is recovered here. For CdS we found that the HOMO was delocalized over the complete cluster, whereas the LUMO was centered to few atoms near the surface. Accordingly, only the LUMO energy was oscillating as a function of cluster size, whereas the HOMO energy was a smooth function. For InP both orbitals

were centered on atoms near the surface. Here, for CdSe, we find in most cases that, as for CdS, the HOMO is spread out over most of the cluster, whereas the LUMO is a surface orbital and, accordingly, the energy of the LUMO is a non-smooth function of cluster size, whereas the energy of the HOMO is a smooth function.

Figure 5 indicates a HOMO-LUMO energy gap of slightly less than 2 eV, i.e., comparable to the experimental value for crystalline CdSe of somewhat less than 2 eV. It should, however, be noticed that density-functional calculations usually lead to too small band gaps, but also that the gap increases rapidly as a function of decreasing size of such nanoparticles. The latter has, e.g., been discussed by Brus[28,29] who showed that when passing to crystallites with a diameter of 2 nm or less (corresponding to the size of the systems of the present study) the lowest exciting energy for such AB semiconductors will increase by from 1 to several eV. Also Yokojima et al.[37] found a significantly increased HOMO-LUMO energy gap for small CdSe particles. In experimental studies, excitonic excitations play a very important role as the lowest-energy excitations. Theoretical calculations of those[30,31,37,43] show that their energies also increase rapidly with decreasing size, as also seen in the experimental studies.[60,61] On the other hand, in their density-functional study of very small CdSe clusters, Troparevsky and Chelikowsky[44] found HOMO-LUMO energy gaps around 2 eV, which was also found by Deglmann et al.[46]

In order to arrive at a qualitative description of the distribution of the various orbitals, we define a radial density as follows. With N_{ij} being the Mulliken gross population for the jth atom and ith orbital we define the density

$$\rho_i(\vec{r}) = \sum_j N_{ij} \left(\frac{2\alpha}{\pi} \right)^{3/2} \exp[-\alpha(\vec{r} - \vec{R}_j)^2], \qquad (4)$$

with α being a chosen, fixed constant. Subsequently, we calculate the spherical average of this density, which is shown in Fig. 6 for i being the HOMO or LUMO. From the figure it is seen that the HOMO is localized throughout the whole cluster and the LUMO is localized at the surface, although, in particular, for the rocksalt-derived clusters some differences show up. When the LUMO is a surface state, its energy
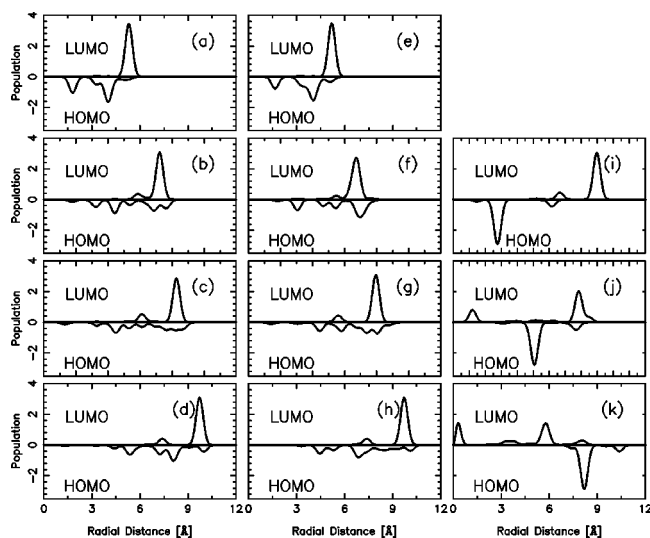
FIG. 6. Schematic representation of the radial distribution of the HOMO and the LUMO for the same clusters as in Fig. 2, i.e., zinc-blende- (left column), wurtzite- (middle column), and rocksalt-derived clusters (right column) of different sizes: (a), (e) $Cd_{16}Se_{16}$; (i) $Cd_{35}Se_{35}$; (b), (f) $Cd_{37}Se_{37}$; (c), (g), (j) $Cd_{58}Se_{58}$; and (d), (h), (k) $Cd_{83}Se_{83}$.

depends sensitively on the cluster surface. Moreover, the difference in spatial distribution of HOMO and LUMO is important for low-energy transitions and is in agreement with the recent experimental results of Lifshitz *et el.*[62,63] on CdSe clusters as well as with the theoretical results of Hill and Whaley.[35,36]

Most experimentally synthesized clusters are nonstoichiometric. Therefore, we have extended our study by also considering nonstoichiometric clusters. We only considered zinc-blende-derived clusters obtained as a spherical part of the zinc-blende crystal structure but with the center at either a Cd or a Se atom. Thereby, the outermost atoms are all of
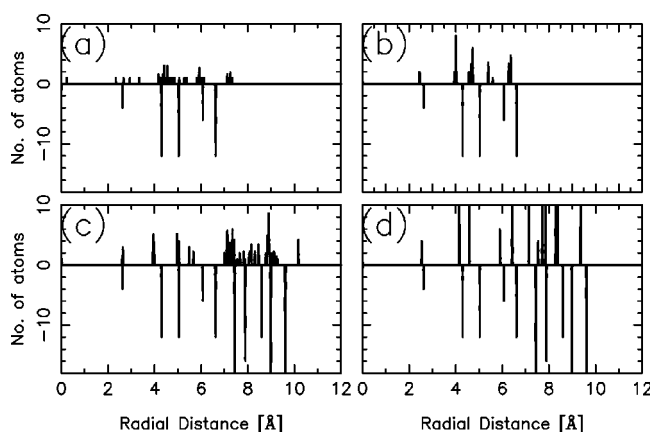

FIG. 7. Radial distribution of Cd and Se atoms for nonstoichiometric Cd-rich (left column) and Se-rich (right column) clusters of different sizes: (a) $Cd_{28}Se_{19}$, (c) $Cd_{79}Se_{68}$, (b) $Cd_{19}Se_{28}$, and (d) $Cd_{68}Se_{79}$. The upper part of each panel shows the structure after relaxation and the lower part the unrelaxed structure, respectively. The radial distance is defined through Eq. (3), and the y axis gives the number of atoms with a certain radial distance.
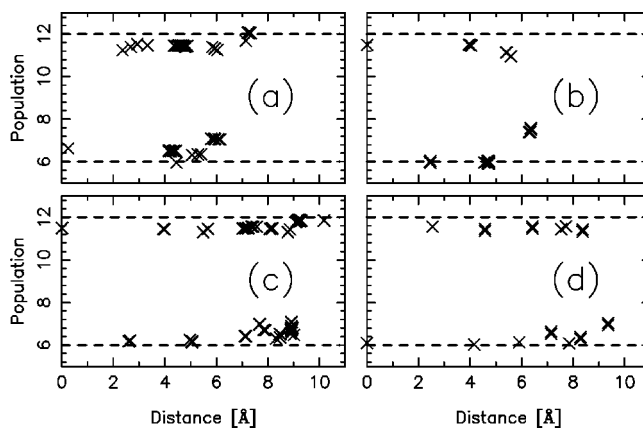
the same type. Moreover, in our analysis we shall distinguish between Cd-rich or Se-rich clusters. Notice that due to our procedure Cd-rich (Se-rich) clusters have Cd (Se) atoms as the outermost atoms.

Due to the differences in the stoichiometries it is not obvious how to compare the total energies of different nonstoichiometric clusters. Therefore, no such comparison is presented. Instead we proceed by analyzing the radial distribution of the atoms and of the Mulliken gross populations, shown in Figs. 7 and 8, respectively. In contrast to the stoichiometric clusters, here the existence of a surface layer characterized by a larger electron transfer between Cd and Se can only with difficulties be identified; instead there is a somewhat scattered population for both types of atoms. Moreover, the structural relaxations are spread out over the complete cluster. For these nonstoichiometric clusters where the outermost atoms are of only one type, the tendency of the chalcogen atoms to move outward and of the metal atoms to move inwards upon structural relaxation, as found for the stoichiometric clusters, is not recovered here.

Both for the Cd- and Se-rich clusters the HOMO-LUMO gap is very small which is very clearly observed in the density of state (Fig. 9). For these cases, the HOMO and LUMO are distributed to the outer parts of the clusters (cf. Fig. 10).
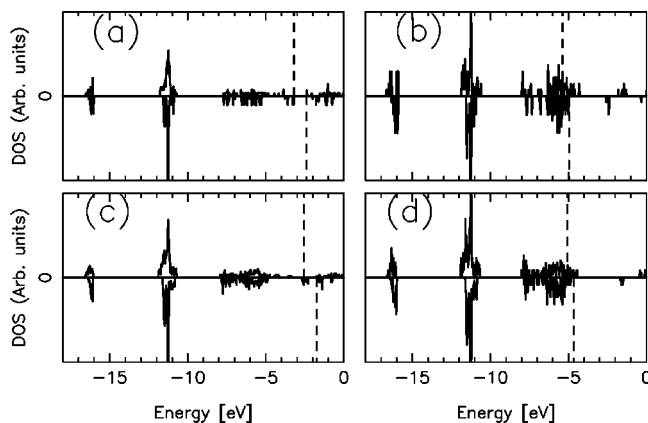

FIG. 8. Radial distribution of Mulliken gross populations for the same clusters as in Fig. 7 in a presentation similar to that of Fig. 3.

FIG. 9. Density of states for the same clusters as in Fig. 7. Notice that the different panels have different scales on the y axis.
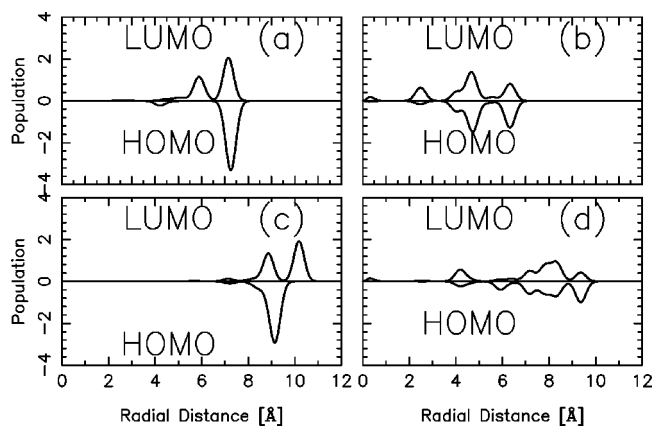
FIG. 10. Schematic representation of the radial distribution of the HOMO and the LUMO for the same clusters as in Fig. 7.

For the stoichiometric clusters we observed an electron transfer in the outer regions corresponding to somewhat less than two electrons donated by the Cd atoms to the Se atoms, which in total resulted in a situation where the Fermi level occurred in a fairly large energy gap. For the nonstoichiometric clusters, a somewhat similar electron transfer is observed (with, however, modifications; cf. Fig. 8), but although the overall shape of the density of states remain unchanged (cf. Fig. 9), the Fermi level occurs now outside the large-gap region. This means that a surface passivation that will recover the behavior of the stoichiometric clusters (i.e., a transfer of somewhat less than two electrons between Cd and Se in the outermost regions) is needed in order to obtain a large-gap cluster, and, accordingly, due to the HSAB principle, a particularly stable structure.

IV. CONCLUSIONS

We have presented results of a theoretical study devoted to both structural and electronic properties of a whole series of stoichiometric and nonstoichiometric naked Cd_mSe_n clusters. Due to the computational demands of a such study, we were forced to employ two fundamental approximations: first, we used a parametrized, non-self-consistent electronic-structure method and, second, we assumed that the structure of the clusters were related to spherical parts of the wurtzite, the zinc-blende, or the rocksalt crystal structure.

Checking the computational method on the infinite crystals led to structural results in good agreement with available information. Subsequently, we found that the zinc-blende- and the wurtzite-derived stoichiometric clusters were ener-

getically close with an important size dependence of their relative stability. As for the infinite crystals, the rocksalt-derived clusters were less stable. The Mulliken gross populations as well as the structural relaxations could be used in identifying a surface layer of roughly 2.5–3 Å. Moreover, in this surface region somewhat less than two electrons per atom were transferred from Cd to Se. As earlier for InP and CdS we found a close correlation between large HOMO-LUMO energy gap and stability, but we stress that the relative stability of zinc-blende- and wurtzite-derived clusters depends not only on the size but also on the material. As for CdS, the HOMO was spread out over the complete cluster for the zinc-blende- and wurtzite-derived clusters, whereas the LUMO was a surface state, whereas for InP both orbitals are surface orbitals. For the rocksalt-derived clusters of CdSe some deviations from this behavior were observed.

Our HOMO-LUMO energy gap is comparable to the value for the crystalline compounds, which can be ascribed quantum-size effects in combination with the well-known underestimate of the band gap in density-functional calculations.

For nonstoichiometric clusters we found a significantly smaller value of the gap, mainly due to the lack of above-mentioned transfer of somewhat less than 2 electrons per atom from Cd to Se. We suggest that, in particular, for these clusters surfactants that passivate dangling bonds and in effect lead to the "ideal" electron transfer are important to stabilize them. But also for the stoichiometric clusters, surfactants that bind to the Se atoms (which are the ones that define the outermost atoms) may stabilize them.

Finally, although this study suffers from some shortcomings, i.e., the lack of surfactants and of a solvent, the simplified, non-self-consistent computational scheme, and the initial assumptions about the structure, it is one of the first systematic studies of a large class of also large clusters, where also structural properties have been addressed. Thus, although it cannot answer all questions definitely, we believe it to be an important contribution to the understanding of the properties of semiconductor nanoparticles, in general, and nanocrystalline CdSe, in particular.

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