

Quasi-Classical Analysis of Boron-Nitrogen Binding

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ABSTRACT: Using the quasi-classical approach the binding energy E of boron-nitrogen system is calculated in dependence of $B-N$ bond length d . Analysis yields the equilibrium values $\langle r \rangle = 1.55 \text{ \AA}$ and $E_{\text{max}} = 4.5 \text{ eV}$, which are in agreement with experimental data available for BN diatomic molecule. The constructed $E=E(d)$ curve is useful for estimations of boron nitride fullerene-like, nanotubular, sheet, and crystalline ($h-BN$, $c-BN$, $w-BN$) structures cohesion parameters as well.

1. INTRODUCTION

Boron nitride (with the chemical formula BN) can be found in form of one-dimensional diatomic molecule, two-dimensional fullerenes and nanotubes, and three-dimensional crystalline (layered hexagonal, cubic zinc-blende, and wurtzite-like) modifications. Crystalline and nanoscale boron nitrides are materials with a diversity of industrial applications. The BN molecule exists only under the extreme conditions, but it also is of special scientific interest being the 'building block' for two- and three-dimensional boron nitride structures.

From the standard thermochemical data the energy of $B-N$ bonds at the equilibrium bond length is known to be considerably stronger in comparison with those of $B-B$ and $N-N$ bonds. Besides any stable boron nitride structure consists of a network of rings with alternating atoms such that the nearest-neighbor environment of boron and nitrogen atoms consists of only $B-N$ bonds. Therefore, $B-N$ bond length is a key interatomic distance in the analysis of boron-nitrogen binding.

In this paper we present the theoretical (namely quasi-classical) method and calculation of $B-N$ interatomic binding energy E in dependence of bond length d , and show that constructed $E=E(d)$

curve is useful for estimations of boron nitride crystalline structures cohesion parameters as well.

2. QUASI-CLASSICAL METHOD

The quasi-classical formula for bounded states energies yields that for substance (i.e. atomic, molecular, and crystalline) inner potentials the precise and quasi-classical electronic spectra are close to one another. On this basis the quasi-classical method of calculation of molecular and crystalline electronic structures and binding energies has been elaborated (its full description one can see in (Chkhartishvili, 2003)).

In the quasi-classical limit the charge density $\rho_{(A)}(r)$ and potential $\varphi_{(A)}(r)$ distributions in (A)-atom are expressed by the step-like functions:

$$\rho_{(A)}(r) = \rho_{(A)i} \quad r_{(A)i-1} < r < r_{(A)i} \quad (i = 1, 2, 3, \dots, q_{(A)}),$$

$$\varphi_{(A)}(r) = \varphi_{(A)i} \quad r_{(A)i-1} < r < r_{(A)i} \quad (i = 1, 2, 3, \dots, q_{(A)}).$$

Here r is the distance from the center of atom; $\rho_{(A)i}$ and $\varphi_{(A)i}$ are the known constants that depend on the nucleus and electrons classical turning points radii $r_{(A)i}$; $q_{(A)}$ is the number of 'homogenous' spherical layers in atom. The radius $r_{(A)i}$ at $i=q_{(A)}$ denoted as \hat{r} is the quasi-classical atomic radius. Applying the Coulomb-like effective potentials affecting electrons and fitting quasi-classical

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energetic spectrum to the Hartree-Fock one we obtained the quasi-classical parameters for boron (B) and nitrogen (N) atoms. The values have been presented in (Chkhartishvili, 2004a).

The quasi-classical adiabatic binding energy •

$$E(d) = \frac{\pi}{3} \sum_{i=1}^{q_{(B)}} \rho_{(B)i} \varphi_{(B)i} (r_{(B)i}^3 - r_{(B)i-1}^3) +$$

$$+ \frac{\pi}{3} \sum_{j=1}^{q_{(N)}} \rho_{(N)j} \varphi_{(N)j} (r_{(N)j}^3 - r_{(N)j-1}^3) -$$

$$- \frac{1}{4} \sum_{i=1}^{q_{(B)}, q_{(N)}} \rho_{(B)i} \varphi_{(N)j} V_{(BN)ij}(d) -$$

$$- \frac{1}{4} \sum_{j=1}^{q_{(N)}, q_{(B)}} \rho_{(N)j} \varphi_{(B)i} V_{(NB)ji}(d)$$

of B-N diatomic system as a function of bond length d is calculated using universal geometrical function $V(R_i, R_j, D)$, which expresses the dependence of the two spheres' intersection region volume upon their radii R_1 and R_2 and intercentral distance D ,

$$V_{(BN)ij}(d) = V(r_{(B)i}, r_{(N)j}, d) +$$

$$+ V(r_{(B)i-1}, r_{(N)j-1}, d) -$$

$$- V(r_{(B)i}, r_{(N)j-1}, d) -$$

$$- V(r_{(B)i-1}, r_{(N)j}, d).$$

Applying the bases set consisting of only outer valence orbitals B-2p and N-2p the BN molecule (i.e. isolated B-N bond) ionization potential IP can be calculated as

$$IP = - \frac{H_{BB} - 2S_{BN}H_{BN} + H_{NN}}{2(1 - S_{BN}^2)} +$$

$$+ \sqrt{\frac{(H_{BB} - 2S_{BN}H_{BN} + H_{NN})^2}{4(1 - S_{BN}^2)^2} + \frac{H_{BN}^2 - H_{BB}H_{NN}}{1 - S_{BN}^2}}$$

where S_{BN} is the overlap integral and H_{BB} , H_{BN} , and H_{NN} denote the molecular Hamiltonian matrix elements. Within the initial quasi-classical approximation they also are expressed by the parameters $r_{(B)i}$, $r_{(N)j}$, $\varphi_{(B)i}$, $\varphi_{(N)j}$, and F-function.

3. BINDING ENERGY CURVE AND IONIZATION POTENTIAL FOR ISOLATED BORON-NITROGEN BOND

The quasi-classically obtained B-N binding energy as a function of interatomic distance reveals the standard behavior characteristic for central pair potentials. $-E(0) = \infty$ and $E(d) = 0$ if d is equal or

more than sum of atomic radii: $d \geq r_{(B)} + r_{(N)}$, while within the intermediate region $0 < d < r_{(B)} + r_{(N)}$ it is an oscillatory function with the several maxima. Among them only one is kinetically available and therefore corresponds to the equilibrium. The piece of $E = E(d)$ curve (in the vicinity of this maximum) is presented in Fig.1. Its analysis yields the values of bond length $d_{max} = 1.55 \text{ \AA}$ and binding energy $E_{max} = 4.51 \text{ eV}$ for BN diatomic molecule. The same dependence determined by us previously (Chkhartishvili et al., 1999) within the frames of another quasi-classical parameterization scheme (for this purpose the screening factor of the potential affecting the given electron in interacting atoms was approximated by the radial polynomial) is relatively flat and leads to estimations of $d_{max} = 1.58 \text{ \AA}$ and $E_{max} = 4.79 \text{ eV}$.

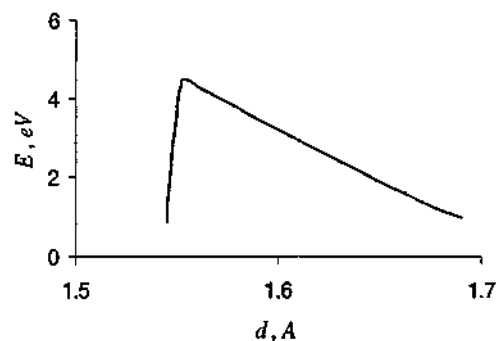


Figure1. Quasi-classically calculated boron-nitrogen binding energy versus interatomic distance in the vicinity of equilibrium

There are known some other first-principles and semiempirical investigations for boron-nitrogen interaction. Applying a self-consistent field procedure to the BN molecule Masse and Bärlocher (1964) calculated molecular orbitals in order to minimize the total energy. Using the spectroscopic data available for this ground state the dissociation energy can be found as 4.6eV. According to the original theoretical approach of Khajt and Baranovskij (1980) the equilibrium interatomic distance in BN molecule equals to 1.307Å The spectroscopic parameters characterizing the calculated boron-nitrogen potential curve lead to the dissociation energy estimation of 5.05eV. A short-ranged classical force-field modeling of boron nitrides has been derived by Marian et al. (2000) on

the basis of experimental and first-principles solid state and diatomic molecular data. Assuming that correct force-field is a sum of only two-body interaction terms, the *B-N* potential energy term has been expressed analytically via Morse potential, which gave $d_{\max}=1.32521\text{Å}$ and $E_{\max}=5.50007\text{eV}$. Pokropivny et al. (2000) emphasized that usual (Morse, Mee-Grüneisen, Buckingham, and other) potentials converge very slowly and hence, a cutoff procedure should be used, but in such case artificial jumps in potential energy and force can be arise. To eliminate this problem using the embedded atom method they have elaborated the interatomic potential for *B-N* system, which fulfills the conditions for smooth end: the potential function and its derivative vanish at the cutoff radius (note that our quasi-classical *B-N* interatomic potential also automatically fulfills the conditions for smooth end at $d=r^{\wedge}_p+r(N)$). The equilibrium bond length of 1.4457/4 and binding energy of 4.00eV were found to reproduce correctly the relative stability of boron nitride layered structures.

The result of present quasi-classical study and previous calculations show that spread in theoretical and semiempirical values for *BN* molecule binding energy (4.0+5.5)eK overlaps with the recommended experimental dissociation energy (4.0+0.5)eV (Gaydon, 1947). However *B-N* bond length quasi-classical value and other concerned theoretical and semiempirical data, which lie over the range (1.307+1.580)Å, are overestimated in comparison with experimental bond length of 1.281Å in *BN* molecule (Huber and Herzberg, 1979). The explanation probably is that *BN* molecule has a triplet ground state, but with an exceedingly low-lying singlet state with a longer bond.

The quasi-classical value of the *B-N* bond ionization potential $IP^*=6.2\text{eV}$ we have obtained self-consistently using the equilibrium bond length $d_{\max}=1.55\text{Å}$ found within the same quasi-classical approach. As it is known the work function is a crystalline counterpart of the molecular ionization potential. To the best of our knowledge, there are no experimental data available neither for boron nitride crystalline modifications work functions nor for *BN* diatomic molecule ionization potential itself. It were suggested only semiempirical values of 11.8eV (Doni and Pastori Parravicini, 1969), 11.5eV (Zunger, 1974a), and 10.6eV (Zunger, 1974b)

obtained for sheet *BN* work function; and theoretical estimations of 11.0eV and 10.9eV determined for *BN* molecule ionization potential using SCF MO method (Masse and Bärlocher, 1964) and the quasi-classical approach within the another parameterization scheme (Chkhartishvili et al., 2000) respectively. All of these quantities have the same order of magnitude (>10eV), but somewhat more than the *IP* found in present work. In this connection it would be noted that the earlier calculations were performed employing the experimental values of *B-N* bond lengths in *h-BN* layers or *BN* molecule, i.e. non-self-consistently. According the interpolative conception of Harrison (1980) the bond length dependence of any energetic gap characterizing substance electronic structure may be approximated as $\sim 1/S$. Consequently, non-self-consistent ionization potential of *BN* molecule should be corrected by the factor of $\sim (d_{\text{exp}}/d_{\max})^2$ where $d_{\text{exp}}=1.28\text{Å}$ is the experimental length of the isolated *B-N* bond. For the case of another quasi-classical parameterization scheme ($d_{\max}=1.58\text{Å}$ and $IP=10.9\text{eV}$) it leads to the ionization potential of 7.1eV, which is in better agreement with the new quasi-classical result 6.2eV.

4. BORON-NITROGEN BOND LENGTHS IN BORON NITRIDE CRYSTALS

Boron nitride is known to crystallize in three modifications *h-BN*, *c-BN*, and *w-BN*. Boron and nitrogen atoms are tetrahedrally surrounded in both of denser forms *c-BN* and *w-BN*. However unlike the zinc-blende case, in the wurtzite structure there are two different nearest-neighbor bonds: one along the *c*-direction with bond length *uc* and three equal bonds forming hexagonal layers with the bond length $\sqrt{a^2/3+c^2(u-1/2)^2}$. Here *a* and *c* are the lattice constants, and *u* is the internal parameter (for a stable wurtzite-type structure *cla* ratio and *u* parameter are strongly correlated in such a way that the unequivalent bond lengths are nearly equal, but the tetrahedral angles are distorted). Any constituent atom of *h-BN* crystal may be considered as a threefold coordinated as the chemical binding occurs only within the layers, whereas weak van der Waals forces are mostly responsible for interlayer binding. *h-BN* has a usual 'graphitic' structure with two-layer stacking sequence, but rhombohedral form *r-BN* with a three-layer stacking also exists.

Besides these three-dimensional layered crystals, the nanotubes and fullerenes on the base of *BN* with layering structures (multi-walled tubes and multi-shelled cage molecules) may be prepared. It urges on analysis of hypothetical isolated infinite hexagonal layer, i.e. sheet *BN*, as a ground state of boron nitride two-dimensional structures. The available first-principles and semiempirical calculations and thermochemical experimental data lead to the binding energy values of about (4+7)eV per *B-N* bond for differently coordinated modifications of boron nitride. Such kind of estimations may be considered to be in qualitative agreement with quasi-classically calculated *B-N* bond energy as the ground state energetic parameters are more sensitive to the atomic coordination than structural ones. By reason of this we focus our attention on the differences in the bond lengths values between boron nitride crystalline phases.

In the work of Strout (2000) the three-coordinated B_12N_{12} network of six-membered rings was examined by theoretical means. Namely the total energy calculated using HF approach or DFT in local and gradient-corrected forms was minimized with respect to *B-N* bond lengths. As the B_nN_n 'graphitic' isomer is only a fragment of sheet boron nitride it has the symmetry with unequal bond angles and bond lengths: (1.266+1.283)₄, (1.371-s-1.378)₄, (1.427+1.442)₄, (1.434+1.444)₄, (1.520+1.536)₄, (1.553+1.576)₄. Formerly within the truncated crystal approach Zunger (1974a) employed two semiempirical (standard and iterative extended Hückel) LCAO methods to the two-dimensional hexagonal boron nitride structure and found bond length to be equal to 1.484 or 1.504. But when semiempirical calculations were performed on small periodic two-dimensional cluster of hexagonal boron nitride layer the equilibrium *B-N* distance was computed as 1.4414 (Zunger, 1974b). The finiteness of quasi-classical atomic radii allowed us to obtain the *B-N* bond length of 1.524 for infinite boron nitride sheet applying the initial quasi-classical approximation (Chkhartishvili, 2004b).

The quasi-classical approach using above mentioned another scheme of parameterization employed for the calculation of *h-BN* binding energy zero-point vibration correction somewhat underestimates the intralayer bond length

(Chkhartishvili and Lezhava, 2001). The reason may be lies in that the crystalline equilibrium configuration was selected by the maximizing its static binding energy with respect to layer lattice parameter only, while the interlayer distance was fixed. Summarizing other theoretical and semiempirical results concerning *h-BN* (and *r-BN*) intralayer bond lengths, we can infer that all of them are in agreement with the experimental value of 1.4464 (von Madelung, 1982). For instance, Xu and Ching (1991) have calculated the total energy of *h-BN* crystal as a function of unit cell volume *V* using orthogonalized LCAO method within the LDA. The equilibrium was found at $V/V_{exp}=0.998$, where V_{exp} is the experimental value of *V*. This result corresponds the intralayer *B-N* distance of 1.4384. The calculations of Albe (1997) also were based on DFT within LDA, but PW expansion for PP and wave function was used. The computed total energies and consequently the intralayer bond lengths for *h-BN* and *r-BN* were nearly the same: 1.4414 and 1.4394 respectively. The short-ranged classical force-field modeling of boron nitrides leads to exactly the same intralayer *B-N* bond lengths in both of layered structures: 1.4544 (Marian et al., 2000).

The *B-N* bond length in *c-BN* obtained from LCAO calculations equals to 1.5654 (Blacha et al., 1984). Applying the full-potential linear APW method systematically Park et al. (1987) computed the total energies for different lattice parameters and fitted them with a parabolic curve. The equilibrium bond length was predicted to be of 1.554. The value of 1.58014 was derived from the one-particle KS equations in the LDA (van Camp et al., 1988). Using the total-energy approach within a localized-orbital formalism Knitte et al. (1989) found two theoretical estimations for *B-N* bond static length: 1.5704 and 1.5674. Xu and Ching (1991) calculated the total energy of *c-BN* as a function of crystal unit cell volume using orthogonalized LCAO method within the LDA. The minimal energy corresponds $V/V_{eip}=1.010$. This result means that equilibrium bond length is 1.5714. The self-consistent MT-orbital band-structure calculation was used by Christensen and Gorczya (1994) to investigate the structural properties of *c-BN*. It suggested that *B-N* bond length equals to 1.574. The cohesive properties of cubic boron nitride were calculated by Malatesta et al. (1997) using Monte

Carlo approach. The total energy was given including finite-size corrections and zero-point vibration energy. They found a value of 1.554 for the bond length in *c-BN*. For a most accurate treatment of this wide-gap insulator within LDA Vogel et al. (1997) employed self-interaction-corrected PP together with Gaussian-orbital basis set and found bond length of 1.59Å while in their relaxation-corrected PP calculation *B-N* distance predicted to be of 1.55Å. Albe (1997) applied the DFT formalism within the LDA based on the PW expansion for PP and obtained bond length of 1.556Å. Karch and Bechstedt (1997) also reported calculation of the structural properties for zincblende *BN* using PW PP method within the DFT. The minimization of the total energy with respect to the crystal unit cell volume yielded nearly the same result of 1.555Å. The short-ranged classical force-field modeling of *c-BN* by Marian et al. (2000) predicted the bond length of 1.564Å. Our quasi-classical estimation of *B-N* bond length in *c-BN* is 1.554Å (Chkhartishvili, 2004a). All of these theoretical results are in good agreement with the experimentally determined value of 1.5656Å for bond length in *c-BN* (von Madelung, 1982).

For *w-BN* the *B-N* bond lengths equilibrium values of 1.571-1.591, 1.552Å-1.571Å, 1.563Å-1.582Å, 1.562Å-1.582Å, 1.553Å-1.570Å, 1.552Å-1.573Å, and 1.564Å-1.573Å were found using full-potential linear APW method (Park et al., 1987), self-consistent local density calculations expanding atomic wave functions in terms of Gaussian orbitals (Xu and Ching, 1991), orthogonalized LCAO method within the LDA (Xu and Ching, 1993), self-consistent linear MT-orbital band-structural calculations (Christensen and Gorczya, 1994), the LDA based on the PW expansion for wave functions (Albe, 1997), PP method within DFT (Karch and Bechstedt, 1997), and short-ranged force-field modeling (Marian et al., 2000) respectively. We had quasi-classically calculated the ground state energy of *w-BN* crystal unit cell as a function of lattice constant *a* fixing the ratio of lattice constants and internal parameter at the 'ideal values': $c/a = \sqrt{8/3}$ and $\kappa = 3/8$ (Chkhartishvili, 2002). Consequently, both of obtained bond lengths coincided: 1.556Å. The above listed theoretical values of equilibrium *B-N* distances in *w-BN* are again in good agreement with experimental ones 1.5661-1.586Å (von Madelung, 1982).

5. CONCLUSIONS

The results of the present study show satisfactory accuracy for the quasi-classically determined boron-nitrogen binding characteristics. Data concerned the calculated bond lengths deviations from the measured ones are given in Table 1.

Table 1. Accuracy of Quasi-Classical Approaches to determination of *B-N* bond lengths

Approach Crystal	Isolated Bond	Bond in Structure
Layer of <i>h-BN</i>	7.2%	5.1%
<i>c-BN</i>	1.0%	0.7%
<i>w-BN</i>	1.0%-2.3%	0.6%-1.9%

It reveals that the computing performed for the given crystalline structure improves upon the accuracy of isolated bond analysis. Though, in both of cases the expected errors of the quasi-classical approaches make up a few percent what is quite acceptable for the materials science purposes. Thus, the obtained *B-N* binding curve and its parameters (equilibrium bond length, binding energy, ionization potential) would be useful for investigations of compounds containing boron-nitrogen bonds.

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