Eur. Phys. J. D **21**, 315–322 (2002)
DOI: 10.1140/epjd/e2002-00204-2

THE EUROPEAN PHYSICAL JOURNAL D

DFT studies of ionic vibrations in Na clusters

P.-G. Reinhard[1] and E. Suraud[2,a]

[1] Institut für Theoretische Physik, Universität Erlangen, Staudtstrasse 7, 91058 Erlangen, Germany
[2] Laboratoire de Physique Quantique, Université Paul Sabatier, 118 route de Narbonne, 31062 Toulouse Cedex, France

Received 23 July 2001 / Received in final form 5 July 2002

Abstract. We use time-dependent density functional theory coupled to molecular dynamics for ionic motion to compute the spectra of ionic vibrations in small Na clusters. Comparison with results from the distance dependent tight-binding approach shows good agreement between these two very different methods. We discuss the evolution of the spectra with cluster size and charge and the impact of ionic vibrations on the optical response.

PACS. 36.40.Mr Spectroscopy and geometrical structure of clusters – 36.40.Sx Diffusion and dynamics of clusters – 33.20.Ea Infrared spectra

Numerous studies have been devoted to the analysis of the geometrical properties of clusters, both from the experimental and theoretical sides [1–5]. In the case of metal clusters, the task is particularly involved due to the large number of isomers and the sloppy character of these systems [6,7]. Basic information on the shape may be acceded from the optical response, with the geometry dependent splitting of the plasmon response [6–8]. However, the optical response does not only reflect geometry but also detailed particle hole electronic excitations, which make its analysis very involved. An alternative approach is to analyze the vibration spectra. This is a well-known procedure in molecular physics and it gives, in principle, more directly access to the ionic structure. But the softness of metal clusters raises here an intrinsic difficulty. It is enhanced by temperature effects which easily turn the cluster into liquid state thus suppressing almost any notion of geometrical structure. A careful cooling of the cluster beam nevertheless allows to attain temperatures below typically 100 K, below which small alkaline clusters may behave as rigid molecules and present well defined vibrational spectra. Up to now, to the best of our knowledge, the only resolved vibration spectra exist for the sodium trimer (apart from the well-known Na_2 dimer) [9,10]. One may nevertheless expect in the near future that a better control of temperature in the beam, as well as appropriate experimental techniques can provide more accurate information about the vibration spectra. The situation is, of course, simpler from a theoretical perspective because it is easier to control the various ingredients and observables. Yet, calculations soon require a sizable computational effort with increasing cluster size. There are thus several calculations for the smallest clusters [11–13] but only few large scale surveys [14–16]. It is the aim of this paper to present a theoretical investigation of vibration spectra in Na clusters with an emphasis on global features and trends with mass number, charge and deformation. Our analysis is based on density functional theory following the methods developed for strongly non linear electronic and ionic dynamics [17].

Vibration spectra in clusters are more involved than in small molecules. Increasing the size leads to a basic smearing of the vibration signals due to (i) the large number of isomers involved (particularly in metal clusters) and (ii) to the higher density of vibration levels for large systems. In this first exploration, we do not want to get lost in all the details and rather focus on the analysis of the dominant pattern related to global observables such as multipole moments of the ionic distribution. We shall thus discuss in the following several pattern of multipole vibration spectra of sodium clusters. We shall in particular address in detail the question of the respective roles of electrons and ions, by varying the net charge of the cluster, an effect which for example could not be attacked in the recent systematic tight binding calculations of [15].

The paper is organized as follows: after a rapid sketch of the model we discuss some examples of vibration spectra in medium size sodium clusters. Before concluding we discuss the impact of vibration on the optical response.

1 Model

1.1 Electronic and ionic dynamics

We employ a robust, simple and most efficient version of time-dependent Density Functional Theory (DFT),

---

[a] e-mail: `suraud@irsamc.ups-tlse.fr`

namely time dependent Local Density Approximation (TDLDA) for the electrons, coupled to classical Molecular Dynamics (MD) for the ions, for details see [17]. We use here the exchange-correlation functional of [18] for the LDA.

The interaction between ions and electrons is described by means of a local pseudo-potential which consists out of a sum of two error functions

$$V_{\mathrm{psp}} = -\frac{Ze^2}{r}\left\{c_1 \mathrm{erf}\left(\frac{r}{\sqrt{2}\sigma_1}\right) + c_2 \mathrm{erf}\left(\frac{r}{\sqrt{2}\sigma_2}\right)\right\} \quad (1)$$

with, for sodium, $c_1 = -2.29$, $c_2 = 3.29$, $\sigma_1 = 0.6809a_0$ and $\sigma_2 = 1.163a_0$. This is a rather soft form which is particularly suited for calculations on a spatial mesh. The parameters have been adjusted to both electronic and atomic properties. They have been tuned to provide electronic atomic spectra and bulk properties (equilibrium density, cohesive energy). They also provide reliable electronic excitation energies, particularly for plasmon resonances [20]. We have also checked the properties of ionic motion. The vibrational frequency of the Na_2 molecule comes out very well.

Ionic dynamics is treated at classical level so far. Ions are propagated under their mutual (point-like) Coulomb interactions, together with the electron-ion forces as derived from the pseudo potential. There is no other external force acting on the system. We explore the spectrum by tracing the free oscillations of the system following a dedicated and small initial excitation. The enormous amount of ionic degrees of freedom allows a very broad choice of initial perturbations. The strong mixing of modes, on the other hand, makes the resulting spectra rather insensitive to the actual initialization. We use two different schemes for the initial perturbation: first, stretching of a single ion, and second, starting ionic dynamics from a thermal velocity distribution. We have checked that both initializations yield the same spectra, which means that the observed frequencies are identical. But the relative distribution of strengths can vary for different initial perturbations. Larger clusters ($N > 20$) are initialized exclusively with thermal distribution.

1.2 Numerical approach

The TDLDA equations are solved numerically on an equidistant grid in coordinate space. For that we have two options, a fully three-dimensional (3D) treatment or a two-dimensional (2D) axially symmetric approximation for the electronic mean fields. Although full 3D calculations are nowadays well in reach of numerical feasibility, they are still too expensive for large clusters and for negatively charged systems (which require large numerical boxes). For sake of efficiency and in order to pursue widespread trends, we restrict the electronic dynamics to cylindrical 2D geometry in most cases. This has been shown to provide a robust and reliable approximation to full 3D calculations for the nearly spherical or axial clusters and for the bulk observables considered here [21–23]. We have counter-checked for some clusters close to axial symmetry (Na_6, Na_7^+, Na_9^+) that 2D and 3D results are identical for the considered observables and within the spectral resolution of our studies. Truly triaxial clusters such as Na_{11}^+ or Na_{13}^+ are, of course, treated in full 3D.

The ground state wavefunctions are determined by an accelerated gradient step [24]. In 2D the time-dependent Kohn-Sham equations for electrons are solved with the Peaceman-Rachford step while in 3D a time-splitting technique is employed. A standard Verlet algorithm is used for the simultaneous ionic propagation, which is, of course, treated in full 3D [23]. As electron emission is negligible, we use reflecting boundary conditions throughout. The boxes are chosen large enough so that boundary conditions have no effects on the dynamics (actually a cylinder with length $88a_0$ and radius $40a_0$). More details on this treatment can be found in the recent review [17]. It should be noted that this coupled ionic and electronic dynamics, constitutes a true TDLDA-MD, beyond the usual Born-Oppenheimer (BO) molecular dynamics. It has been widely used in the regime of non-linear dynamics where it is unavoidable to treat electronic and ionic motion simultaneously [17]. It was also checked that the full TDLDA-MD correctly reduces to a Born-Oppenheimer dynamics as long as electrons are only very weakly excited [25]. As our numerical approach is very efficient, we will use the TDLDA-MD here to study ionic vibrations. The full capabilities of TDLDA-MD are required for our final example, the coupling of ionic vibrations to optical response.

1.3 Observables

In very small clusters, each ionic eigenfrequency can be easily identified and attributed to a well defined motion of individual atoms. For larger clusters, the situation becomes soon very intricate and the analysis of eigenfrequencies is easier in terms of multipoles, just as in the case of a continuous medium, like a droplet. We have thus chosen to study ionic vibrations of sodium clusters in terms of the lowest order multipole moments of the ionic distribution, namely the monopole, quadrupole and octupole moments. These corresponds already to $1 + 5 + 7 = 13$ observables. This allows to scan the basic changes of a system: expansion (monopole), deformation (quadrupole), and symmetry breaking (octupole). We simplify the study by considering only the axially symmetric multipole moments. These are sufficiently representative for the nearly spherical clusters. They still give many useful hints for deformed clusters. The axial moments are defined as (up to, here irrelevant, fore-factors)

$$\begin{aligned} q_0 &= \sum_I (X_I^2 + Y_I^2 + Z_I^2) \\ q_2 &= \sum_I (2Z_I^2 - X_I^2 - Y_I^2) \\ q_3 &= \sum_I Z_I(2Z_I^2 - 3X_I^2 - 3Y_I^2) \end{aligned} \quad (2)$$

where the summations run over all ions of coordinates (X_I, Y_I, Z_I). The axes of the reference frame are the principal axes of the ionic distribution. The "Z" axis is the axis of highest (discrete) symmetry in the cluster which coincides in the 2D electronic approximation with the symmetry axis of the electronic wavefunctions as well.

We first prepare the cluster in its ground state configuration. Then we excite the system by a small displacement of one ion or alternatively by a thermal velocity distribution. The slight ionic excitation corresponds to a vanishingly small excitation energy of order typically 10 meV, which is negligibly small at the side of electrons but which matches with typical ionic frequencies. Moreover, we assume that the low multipole moments defined above provide a representative analysis. We have counter-checked that by varying the excitation mechanism as well as the analyzing observables (checking also single ion vibrations). After initial excitation, we then record in time the ionic multipole moments $q_i(t)$ $(i = 0, 2, 3)$. By Fourier transform into the frequency domain we accede $\tilde{q}_i(\omega)$ from which we obtain power spectra as $|\tilde{q}_i(\omega)|^2$ or strengths as $\mathcal{I}(\tilde{q}_i(\omega))$, which will be our basic observables for forthcoming discussions of results. It should be noted that this spectral analysis proceeds here exactly as in our systematic studies of optical response, at the electronic side [17,26]. The optical spectra shown at the end of this paper will actually be computed in a similar fashion. The initialization is then done at the electronic side by a small boost of the electron cloud. And we additionally take a protocol of the electronic dipole momenta to explore the electronic spectra of the cluster.

2 Results

2.1 Ground state properties and first tests

Before considering systematic calculations of vibration spectra, we want to check the validity of our method, particularly with respect to ionic structure and vibration properties. We first consider the simplest case of the sodium dimer Na_2 for which these properties are well established both experimentally and theoretically. Our TDLDA calculations lead to a dimer bond length $d = 5.71a_0$ to be compared to the experimental value $d = 5.82a_0$. Ionization potentials (IP) provide a further insight into the structure. To that end, we employ a self-interaction correction (SIC), which is treated here according to the recipe of [19]. This allows to compute the IP from the energy of the last occupied electron state. The theoretical value is $IP = 4.93$ eV which again compares very well with the experimental $IP = 4.90$ eV. Finally the molecular vibration frequency probes the curvature of the inter-atomic potential and provides a validity check for our systematic calculations of ionic frequencies. We obtain a theoretical frequency of 165 cm^{-1} (20.5 meV) to be compared to the experimental value of 159 cm^{-1} (19.7 meV). Again the comparison indicates that our approach is sufficiently reliable.

The structure of systems larger than Na_2 is best explained graphically. To that end, we show in Figure 1 the set of (LDA) ionic structures used in the calculations for this paper. The figure is self-explaining.

Results on ionic vibrations of clusters heavier than Na_3 are not numerous. It is nevertheless interesting to compare our results to the ones obtained recently by means of a BO Molecular Dynamics based on a tight binding Hamiltonian [14,15]. The distance dependent tight binding (DDTB) Hamiltonian used in these calculations has proven to provide a reliable tool of investigation of ionic structures of simple sodium clusters [27]. The ionic structures obtained from DDTB perfectly match with the CAPS ones for all axial clusters [21]. We check here the agreement for ionic vibration spectra. The comparison is performed in Figure 2 in terms of our basic multipoles for ground state Na_6. At first glance, one observes a remarkable agreement between the two calculations. The two observed frequencies coincide. Even the relation of strengths is comparable for the monopole and quadrupole. At second glance, one can note a few differences. The widths of the peaks are larger in TDLDA-MD which is a trivial numerical effect from different observation time (4 ps in TDLDA-MD *versus* 20 ps in DDTB-MD). The relation of strengths for the octupole is exchanged. This is most probably an effect from different initialization of the ionic oscillations. They are initialized in DDTB-MD from infinitesimal heating of the whole cluster (temperature of about 10 K) while TDLDA-MD starts from zero temperature ground state and starts from stretching the top ion a bit along the symmetry axis (leading to an average excitation of about 1 K). Altogether, the comparison confirms that our TDLDA-MD calculations rely on safe grounds also for studies of ionic vibrations. We have also checked the 2D approach by comparing with 3D DFT results for the case of Na_7^+. We find again a very good agreement.

The ionic spectra of Na_6 (Fig. 2) display a pronounced double hump structure in all three collective observables. This effect is linked to the actual ionic structure of Na_6 made of a ring of 5 ions topped by a single ion, see Figure 1. By detailed analysis of separate ions, we have found out that the two dominant modes are a breathing of the ring and an oscillation of the top ion relative to the ring. These two modes couple to yield the final two peaks and they have a component in each global moment, monopole, quadrupole and octupole.

2.2 Vibration spectra of medium size charged clusters

We now proceed to systematic studies which include also charged clusters. Note that such calculations could not be attacked in former DDTB calculations. This is an important aspect, both because charged clusters are easier to handle experimentally and because this allows us to study the impact of net charge (defect or addition of electrons) on ionic vibrations. Figure 3 shows a systematic study of size dependence for positively charged clusters. We have chosen here a set of nearly spherical clusters, see left column in the figure, to see the size dependence. Effects of

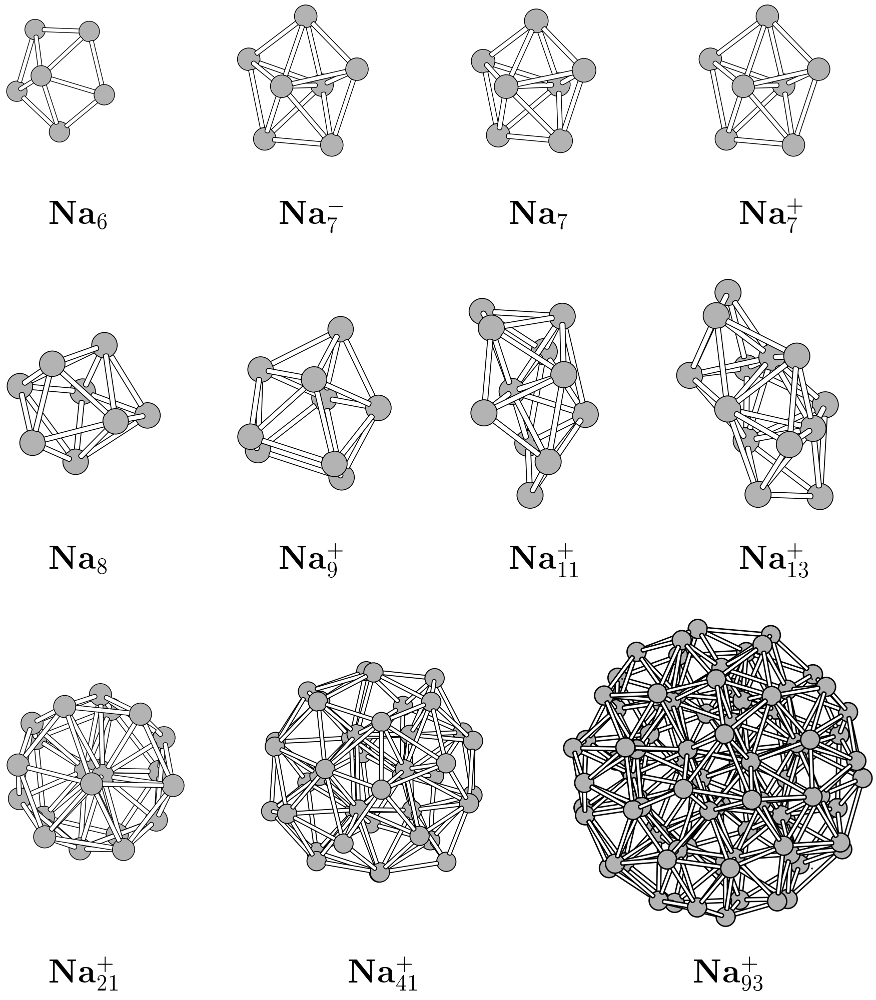

Fig. 1. Calculated LDA ionic structures of the various clusters considered in this paper.

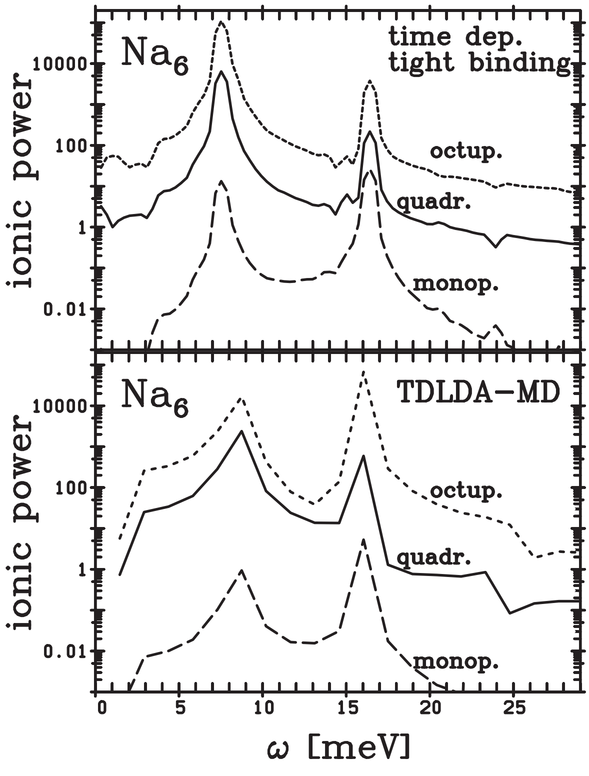

Fig. 2. Power spectra of ionic motion for the cluster Na$_6$ and for the three basic multipolarities (monopole = dashed, quadrupole = full line, octupole = dotted). Compared are results from DDTB-MD (upper panel) and TDLDA-MD (lower panel).

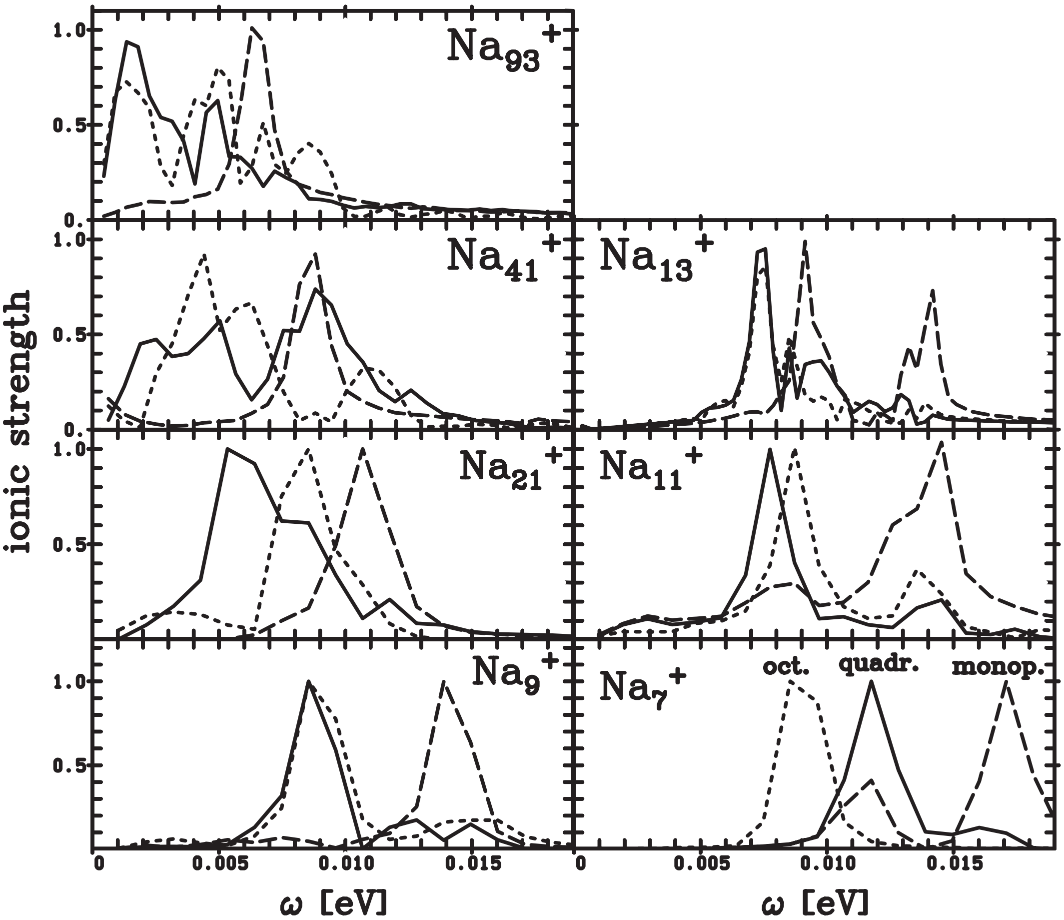

Fig. 3. Strength of ionic motion for the three basic multipolarities (monopole = dashed, quadrupole = full line, octupole = dotted). The various panels show results for different positively charged clusters. The left column shows a sequence of nearly spherical clusters. The right column shows a few deformed systems, nearly axially symmetric Na_7^+ as well as triaxial Na_{11}^+ and Na_{13}^+.

deformation are demonstrated by the complementing samples in the right column. Let us first concentrate on the nearly spherical clusters shown in the left column. The global trend is a decrease of frequencies with increasing cluster size. That is similar to what is observed in liquid-like droplets such as atomic nuclei [28]. Within this global trend, the relative positions of the multipolarities vary from one cluster to the next. The monopole is the cleanest mode of all following nicely a trend $\sim 0.03\,\mathrm{eV}\,N^{-1/3}$. Quadrupole and octupole modes show also the general decrease $\propto N^{-1/3}$. But these modes are more and more fragmented the larger the clusters so that the lower end of the spectra drops more quickly than $N^{-1/3}$.

The deformed systems, shown in the right column of Figure 3, add a new aspect. The smallest and still rather rigid case Na_7^+ lines up nicely with the spherical sequence. The two other examples are electronically soft (a typical feature of triaxial clusters). As a consequence, the spectra are a bit more diffuse already for small clusters and there is a tendency to deviate from the above stated trends. Even the "robust" monopole mode can be fragmented (see Na_{13}^+). The quadrupole mode is lower than in comparable spherical systems. This is related to the known quadrupole softness of these triaxial systems.

2.3 Respective roles of ions and electrons

We now turn towards the question of the impact of cluster net charge on ionic vibrations. We do this in two ways. First, we fix the number of electrons at the magic value 8 and vary the number of ions. We thus consider the set of three clusters Na_7^-, Na_8, Na_9^+. It should be noted that we are comparing here three clusters with similar electronic properties but different numbers of ions, hence with somewhat different ionic structures. Indeed, while Na_7^- exhibits a marked prolate shape with a ring of 5 ions topped by 2 outside plane ions (one on each side), both Na_8 and Na_9^+ ground state structures look more "spherical" (Fig. 1). Results are presented in Figure 4, where we compare the vibration spectra of Na_7^-, Na_8, Na_9^+, in terms of monopole, quadrupole and octupole strengths. The frequencies are stable from one cluster to the next. The overall positions of the 2 dominant peaks are also the same and monopole and octupole modes are, to a large extent, independent

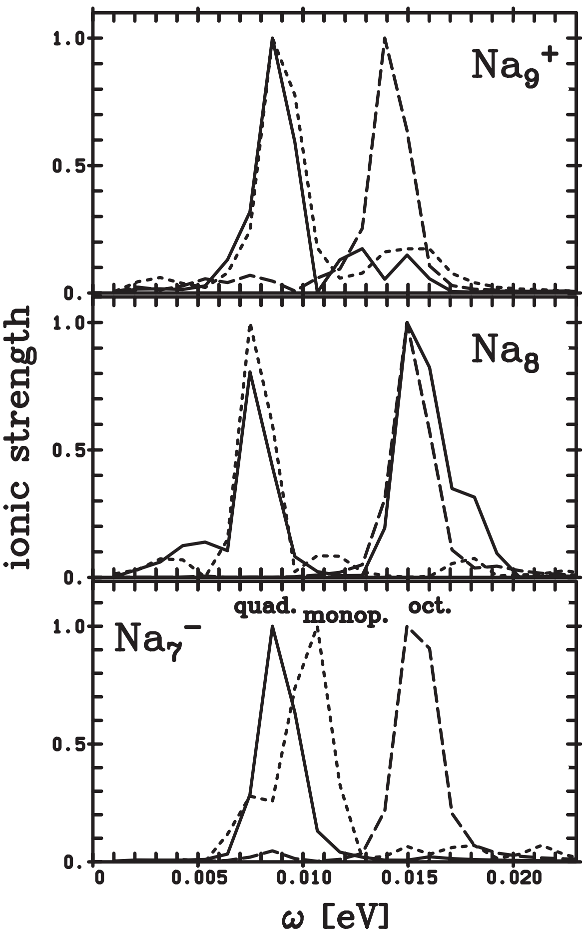

Fig. 4. Power spectra of ionic motion for the three basic multipolarities (monopole = dashed, quadrupole = full line, octupole = dotted). The panels show a variation of cluster size for $N_{\mathrm{el}} = 8$.

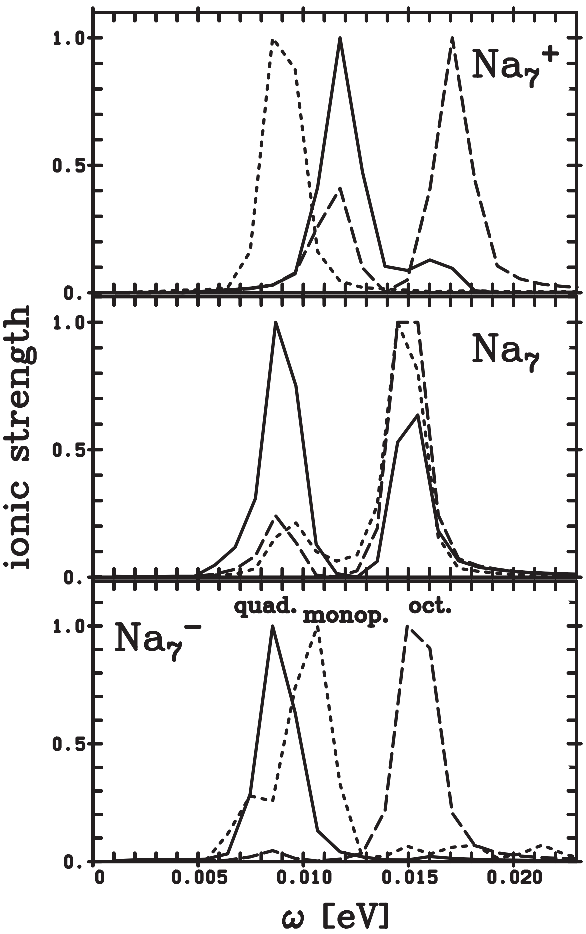

Fig. 5. Power spectra of ionic motion for the three basic multipolarities (monopole = dashed, quadrupole = full line, octupole = dotted). The panels show a variation of cluster charge for $N_{\mathrm{ion}} = 7$.

of the charge. The single "exotic" behavior is here observed for the quadrupole mode, where the distribution of strengths over the two peaks varies from one charge state to the next. The Na_8 case shows two peaks of comparable height while the two other clusters concentrate quadrupole strength at the lower peak. Altogether, we nevertheless observe here relatively stable spectra when changing the net charge at fixed electron number.

In order to complement the former analysis, we now fix the number of ions and vary the number of electrons. We thus consider the set of three clusters Na_7^-, Na_7, Na_7^+. In this case the three considered clusters have basically the same ionic structure (Fig. 1), only the net charges differ. Results are displayed in Figure 5. The figure exhibits some similarities and differences with Figure 4. First, one observes again rather stable frequencies, although there is a faint trend towards larger frequencies with increasingly positive net charge. This is at variance with the previous case of fixed electron number in which the tendency, if any, was the other way around. Again we note a specific behavior of the quadrupole frequency which exhibits a marked double hump structure for the neutral species Na_7, just as in Na_8 (Fig. 5). In the present case, still, the effect is also clearly visible in both monopole and octupole signals, just as was found in Na_6 (Fig. 2). This may suggest a systematic trend which should be explored in a more systematic way. After all, there are only small changes with changing charge while frequencies shrink generally $\propto N^{-1/3}$ with changing size N.

2.4 Ionic versus electronic vibrations

The TDLDA-MD with its coupled electronic and ionic dynamics allows to investigate the dynamical interplay between ionic vibration and the optical response of a metal cluster. Note that there are two effects of ionic vibrations on the electronic spectra: the thermal line broadening and the dynamical coupling. The thermal effect produces an ensemble of ionic configurations which explore the Born-Oppenheimer surface at thermal energies. Optical absorption measurements take snapshots of these various configurations and add up the slightly different spectra incoherently to one broadened peak. This mechanism was much studied in the past, see *e.g.* [29–32]. The crucial role of octupole softness was pointed out in [31,32]. A different

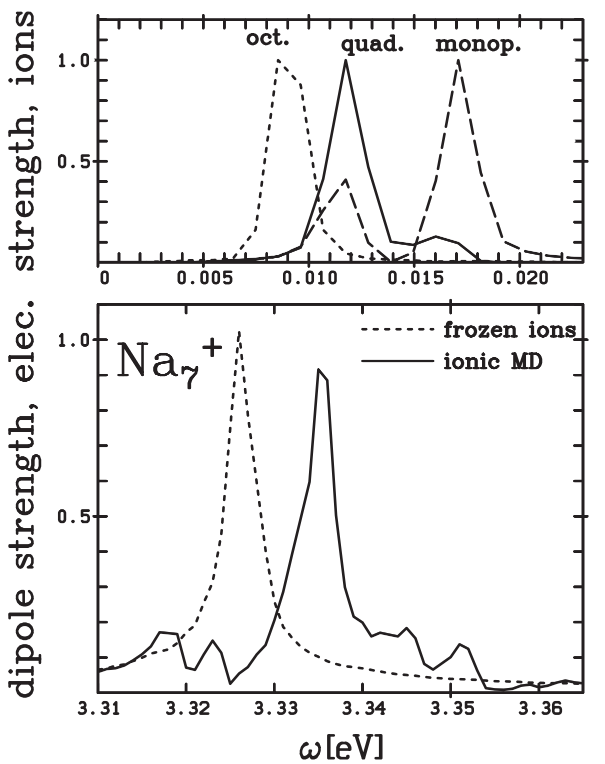

Fig. 6. Ionic and electronic power spectra for Na_7^+. The upper panel shows the ionic spectra for the three basic multipolarities (monopole = dashed, quadrupole = full line, octupole = dotted). The lower panel shows the electronic dipole power in a narrow window around the peak for the resonance mode along symmetry axis. The full line shows the result from full TDLDA-MD. The dotted line comes from a similar calculation with frozen ionic configuration.

mechanism is at work in the dynamical coupling. Here one considers a coherent superposition of electronic and ionic vibrations. This is comparable to dynamical phonon coupling in solids or coupling of giant resonances and surface modes in nuclei [28]. In the following, we are studying this second effect, the dynamical coupling to ionic vibrations, which requires full TDLDA-MD.

The electronic oscillation is here excited by a simple initial boost of the whole electron cloud. The boost induces an excitation energy of less than 0.1 eV and is small enough to ensure that we remain deeply in the linear domain of electronic excitations. In order to analyze the impact of ionic vibrations on the optical response we perform two calculations, one with fixed ionic background and another one with full ionic motion taken into account. Results are displayed in Figure 6. The upper panel of the figure recalls the ionic vibration spectra as discussed above. The lower panel shows the optical responses for fixed and for moving ions. The two optical spectra are practically the same when viewed at a coarse scale. But they exhibit interesting differences in detail. First, the peak with ionic MD is about 10 meV higher than without ionic motion, which is the typical range of ionic vibrations (see upper panel). This is exactly the up-shift one would expect from a simple classical model of two coupled oscillators (one for the ions, one for the electrons). The second difference lies in the forms of the spectra in the immediate vicinity of the main peak. The full calculation with ionic motion exhibits a series of side peaks located again in a range of order 10 meV around the major peak. It is very likely that we again see here the spreading of the plasmon due to coupling to the phonons. The energetic range of the spreading fits nicely with the vibration spectra shown in the upper panel of Figure 6. But note that the coupling is rather low such that the FWHM of the resonance is not significantly changed by the phonons.

3 Conclusions

In this paper we have analyzed the vibration spectra of simple metal clusters in terms of multipole moments. For this purpose, we have used our well documented TDLDA-MD description of electron dynamics within TDLDA, coupled to ionic molecular dynamics (MD). The TDLDA-MD results agree quantitatively with former DDTB-MD calculations. We have systematically explored the impact of charge, system size, and the interplay of electronic and ionic effects on vibration spectra. The size dependence is mixed. Clusters with comparable gross properties (here all spherical) produce a trend $\propto N^{-1/3}$ in the vibration frequencies. Deformation seems to induce fluctuations about this global trend, particularly for octupole and monopole modes. We could not find any significant dependence on the net charge of the cluster. Finally, we have explored the interplay between electronic and ionic degrees of freedom around the most dominant electronic excitation, the Mie plasmon peak. One sees the spreading of the plasmon through phonons. But the coupling is very weak and has little effect on the plasmon width. The experimental access to vibration spectra in metal clusters is not easy. With the TDLDA-MD it might nevertheless be possible to investigate practical ways to perform such studies for example by exploring the impact of vibrations on photo-electron spectra. Work along this line is in progress.

The authors thank the French-German exchange program PROCOPE number 99074 and Institut Universitaire de France for financial support during the realization of this work.

References

1. T.P. Martin, Phys. Rep. **273**, 199 (1996)
2. T. Baumert, G. Gerber, Adv. At. Mol. Opt. Phys. **35**, 163 (1995)
3. *Large clusters of atoms and molecules*, NATO ASI **E313**, edited by T.P. Martin (Kluwer, Dordrecht, 1996)
4. Special issue “Small Particles and Inorganic Clusters”, ISSPIC 9, edited by A. Châtelain, J.-M. Bonnard, Eur. Phys. J. D **9** (1999)
5. V. Bonačić-Koutecký, P. Fantucci, J. Koutecký, Chem. Rev. **91**, 1035 (1991)
6. W. DeHeer, Rev. Mod. Phys. **65**, 611 (1993)
7. M. Brack, Rev. Mod. Phys. **65**, 677 (1993)
8. *Cluster of Atoms and Molecules I*, edited by H. Haberland, Springer Series in Chemical Physics (Berlin, 1994), Vol. 52

9. M. Broyer, G. Delacretaz, P. Labastie, J.P. Wolf, L. Woste, J. Phys. Chem. **91**, 2626 (1987)
10. G.H. Jeung, M. Broyer, P. Labastie, Chem. Phys. Lett. **165**, 494 (1990)
11. J.L. Matins, R. Car, J. Buttet, J. Phys. Chem. **78**, 5646 (1983)
12. F. Cocchini, T. Upton, W. Andreoni, J. Phys. Chem. **88**, 6068 (1988)
13. T.C. Thompson, G. Izmirlian, S.J. Lemon, D.G. Truhlar, C.A. Mead, J. Phys. Chem. **85**, 5597 (1985)
14. C.Z. Wang, C.T. Chan, K.M. Ho, Phys. Rev. Lett. **66**, 189 (1991); R. Poteau, F. Spiegelmann, J. Chem. Phys. **98**, 6450 (1993)
15. F.S. Zhang, E. Suraud, F. Calvo, F. Spiegelmann, Chem. Phys. Lett. **300**, 300 (1999)
16. R.S. Berry, B.M. Smirnov, JETP **90**, 491 (2000)
17. F. Calvayrac, P.-G. Reinhard, E. Suraud, C. Ullrich, Phys. Rep. **337**, 493 (2000)
18. J.P. Perdew, Y. Wang, Phys. Rev. B **45**, 13244 (1992)
19. C.A. Ullrich, P.-G. Reinhard, E. Suraud, Phys. Rev. A **62**, 053202 (2000)
20. S. Kümmel, P.-G. Reinhard, M. Brack, Eur. J. Phys. D **9**, 149 (1999)
21. F. Spiegelmann, R. Poteau, B. Montag, P.-G. Reinhard, Phys. Lett. A **242**, 163 (1998)
22. B. Montag, P.-G. Reinhard, Z. Phys. D **33**, 265 (1995)
23. F. Calvayrac, P.-G. Reinhard, E. Suraud, Eur. Phys. J. D **9**, 389 (1999)
24. V. Blum, G. Lauritsch, J.A. Maruhn, P.-G. Reinhard, J. Comp. Phys. **100**, 364 (1992)
25. F. Calvayrac, Ann. Phys. Fr. **23**(3), 1 (1998)
26. F. Calvayrac, P.-G. Reinhard, E. Suraud, Ann. Phys. (NY) **255**, 125 (1997)
27. R. Poteau, F. Spiegelmann, Z. Phys. D **30**, 57 (1994)
28. J. Eisenberg, W. Greiner, *Nuclear Theory I* (North-Holland, Amsterdam 1970)
29. G.F. Bertsch, D. Tomanek, Phys. Rev. B **40**, 2749 (1989)
30. J.M. Pacheco, R.A. Broglia, B.R. Mottelson, Z. Phys. D **21**, 289 (1991)
31. B. Montag, P.-G. Reinhard, Phys. Rev. B **51**, 14686 (1995)
32. M. Moseler, U. Landmann, C. Yannouleas, Phys. Rev. Lett. **87**, 053401 (2001)