# QUANTUM CONFINEMENT OF MOBILE $Na^+$ IONS IN SODIUM SILICATE GLASSY NANOPARTICLES

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**Abstract.** The confinement of mobile $Na^+$ ions in sodium silicate glassy nanoparticles is considered quantum mechanically to be under the influence of a spherical box potential. The values for the energies of mobile $Na^+$ ions are determined theoretically for particle diameters of 1nm, 2nm and 5nm. For 1nm and 2nm particles, for a given value of the principal quantum number 'n', it is shown that the energy level separations between adjacent levels lie in the microwave region of the electromagnetic spectrum.

*Keywords:* glassy nanoparticles; nanostructures; nanostructured materials; amorphous oxides; quantum confinement; spherical box potential

## Introduction

In sodium silicate glasses, $Na^+$ ions are network modifiers (Mehrer et al., 2008). In the ground state they are bound to oxygen anions. When excited either thermally or photolytically (or by particles) they can transition to unbound states as shown in Fig. 1. Sodium cations excited to unbound states are mobile. Now, in a glass particle of macroscopic dimensions, the mobile sodium cations populate a band of quasi-continuous states and drift through the solid. When the size of the glass nanoparticles is shrunk to nanodimensions (typically less than about 5 nm in diameter), the quasi-continuous band of unbound states split into discrete levels as is shown in this paper. In these nanoparticles, excitation of $Na^+$ ions from states where it is bound to oxygen anions to mobile states results in excitation to discrete states as shown in Fig. 1 (b).

In this paper, I throw light on the discrete states to which the mobile $Na^+$ ion is restricted to in sodium silicate glassy nanoparticles. I use the spherical box potential described below to quantum mechanically obtain the energy levels of the mobile $Na^+$ cations restricted to nanometric dimensions. Even though the spherical box potential is an approximation, the type of states that are possible is delineated as glass is an isotropic medium. Transitions from states in which $Na^+$ is bound to oxygen anions to states in which $Na^+$ is mobile may be experimentally validated through spectroscopic studies. It is also the purpose of this paper to act as a stimulus for such studies and, therefore, provide an understanding of the phenomenon in greater depth.

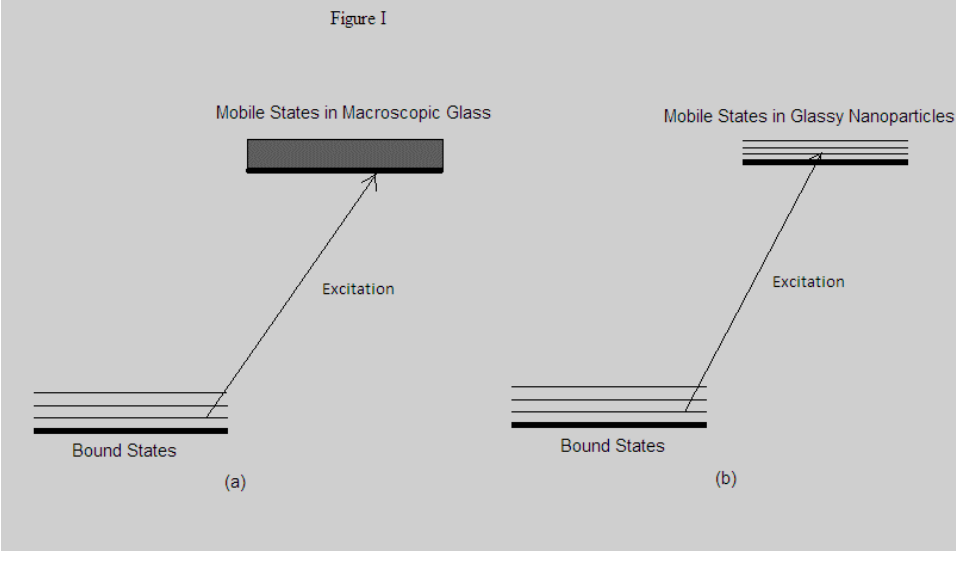


**Fig. 1.** Transition of $Na^+$ cations from bound to mobile states

**Computational procedure**

Mobile $Na^+$ ions are in energy states where they are free to move through the solid until de-excitation puts them back into a bound state. For the purposes of computation, the mobile $Na^+$ are assumed to be free to move within the sodium silicate glassy nanoparticles and are considered to be restricted only by the boundary of the nanoparticle. The nanoparticle is taken to be spherical. Therefore, the confinement of $Na^+$ ions within the glassy nanoparticle is considered quantum mechanically to experience a spherical box potential (Agarwal & Prakash, 1996; Fitzpatrick, 2015) as given by Eq. (1) where '*r'* is the radius variable and *'a'* is the value of the radius of the spherical nanoparticle.

$$V(r) = \begin{cases} 0 \; for \; r \leq a \\ \infty \; for \; r > a \end{cases} \tag{1}$$

Appropriate values of the energies of the Na+ ions in various sizes of glassy nanoparticles are obtained. To my knowledge, the confinement of Na+ ions within glassy nanoparticles has not been considered quantum mechanically in the literature before. That such an approximation is justified is supported by the fact that other physical systems such as f-centers in salt crystals have been modeled by using the particle in a three dimensional box approximation (House, 2005)

The time-independent Schrodinger equation for a particle under the influence of a spherical box potential has been solved previously (Agarwal & Hari Prakash,

1996; Fitzpatrick, 2016) and the expression for the energy of the particle has been obtained as given below in Eq. (2).

$$E_{nl} = \frac{h^2 z_{nl}^2}{8\pi^2 m a^2} \tag{2}$$

In Eq. (2) '*m*' is the mass of the particle and $z_{nl}$ represents the zero roots of $j_l(z)$ where *z* is given by Eq. (3).

$$z=kr, \tag{3}$$

'*k'* is the magnitude of the wave vector and $j_l(z)$ represent the spherical Bessel functions. As can be seen from Eq. (2), the quantum numbers *n* and *l* determine the values of the quantized energy levels.

**Results and discussion**

Table 1 presents the energy levels which have been calculated using equation (2) for $Na^+$ ions in spherical sodium silicate glassy nanoparticles of diameters 1nm, 2nm and 5nm. The values that $z_{nl}$ have is based on those in Agarwal & Prakash (1996).

It can be seen from Table 1 that as n increases the values of the separation between adjacent energy levels also increase. Further, as the diameters of the nanoparticle increases from 1 nm to 5nm, for a given value of n, the $E_{nl}$ values decrease substantially between adjacent energy levels. For a 1nm diameter particle the 1s $\rightarrow$ 1p transition lies at 0.3020 $cm^{-1}$ while the 1s $\rightarrow$ 2p transition lies at1.4628 $cm^{-1}$. These transitions lie in the microwave region of the electromagnetic spectrum which spans the region from 0.033 $cm^{-1}$ to 3.3 $cm^{-1}$ (McQuarrie, 2003). The 1s $\rightarrow$ 1p transition in a 2nm diameter particle lies at 0.0755 $cm^{-1}$ while the 1s $\rightarrow$ 2p transition in nanoparticles of this size lies at 0.3657 $cm^{-1}$. Both these values are in the microwave region. In a 5 nm diameter nanoparticles, the 1s $\rightarrow$ 2p transition lies at 0.0121 $cm^{1}$. This is clearly in the sub-microwave region of the electromagnetic spectrum. The 1s $\rightarrow$ 2p transition, however, lies at 0.0585 $cm^{-1}$ which is in the microwave region.

**Conclusion**

It can be said that the confinement of mobile $Na^+$ ions results in discrete energy levels in the sodium silicate glassy nanoparticles considered here. Spectroscopically, it should be possible to measure the transition of $Na^+$ from states where it is bound to oxygen anions to states where it is mobile as delineated in this report. Further, this result is significant in the sense that these and other metal ion containing glassy nanoparticles can be explored for use in nanoionics among possibly other applications as well.

**Table 1.** Values of $E_{nl}$ for $Na^+$ ions in glassy nanoparticles of different sizes

| | $E_{nl}$ ($10^{-24}$ J) | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| l | n = 1 | | | n = 2 | | | n=3 | | |
| | a (nm) | | | a (nm) | | | a (nm) | | |
| | 0.5 | 1.0 | 2.5 | 0.5 | 1.0 | 2.5 | 0.5 | 1.0 | 2.5 |
| 0 | 5.7421(1s) | 1.4355 | 0.2297 | 22.9686(2s) | 5.7421 | 0.9187 | 51.6793(3s) | 12.9198 | 2.0672 |
| 1 | 11.7411(1p) | 2.9353 | 0.4696 | 34.7996(2p) | 8.6999 | 1.3920 | 69.1939(3p) | 17.2985 | 2.7678 |
| 2 | 19.3223(1d) | 4.8306 | 0.7729 | 48.2278(2d) | 12.0570 | 1.9291 | | | |
| 3 | 28.4557(1f) | 7.1139 | 1.1382 | 63.2340(2f) | 15.8085 | 2.5294 | | | |
| 4 | 38.9692(1g) | 9.7423 | 1.5588 | | | | | | |
| 5 | 51.0231(1h) | 12.7558 | 2.0409 | | | | | | |
| 6 | 64.3310(1i) | 16.0828 | 2.5732 | | | | | | |

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