Capacitance Definition in the Atomic Scale and its Applications

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Abstract: In this letter we introduce the definition of the capacitance in the atomic scale. The capacitance in the atomic scale is the same as the macro scale but the electrodes will be the maximum probability sheets of finding the electron. Based on this definition, an electrical model – equivalent circuit – for atom's emission is presented and Hydrogen atom is taken as an example. The line spectra of Iron and Sodium are used to verify the model. Also the concept of capacitance property is introduced. It means the capacitance between the upper and lower quantum states of the valence and conduction band energies respectively.

PACS numbers: 36.20.Kd 74.25.Jb 73.43.Jn

Keywords- Capacitance, Electron orbital, Atom's emission, Atom's modeling, Band gap materials, Capacitance Property.

The band gap tunability of graphene bilayer structure by applying a voltage difference or electric field on it [1] encourages us to define a new material property which has an electrical interpretation of the phenomenon. So we suggest the capacitance as a new material property.

The capacitance property is an application of *the capacitance definition in atomic scale* or in other words the *capacitance between quantum states*.

To clarify the concept of capacitance between quantum states, we compare the emission of tunnel junction and the emission of an atom. Fig. (1) compares the energy and frequency of the emitted photons from tunnel junction and an atom.

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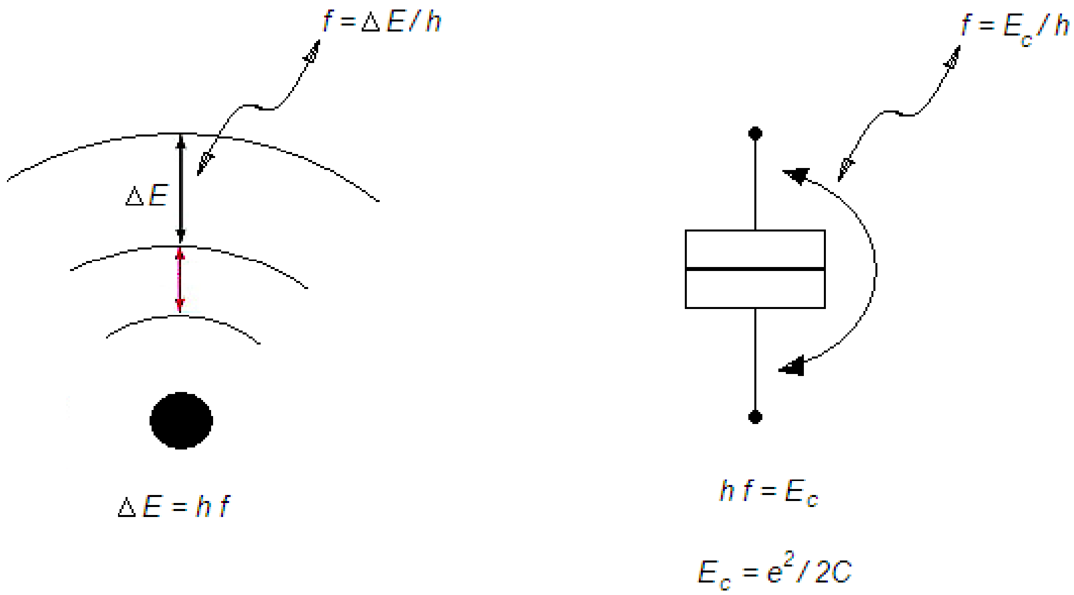

Fig 1. Energy and frequency of the emitted photons from tunnel junction and an atom.

The frequency of the radiated photon from the tunnel junction $f_{TJ}=E_c/h$ [2], E_c is the charging energy,

$$E_C = \frac{e^2}{2C} \tag{1}$$

where e is the electron charge and C is the tunnel junction capacitance. The frequency of the radiated photon from the atom $f_{Atom}=\Delta E/h$.

To complete the analogy, we may assume $\Delta E=E_c$, this means:

$$\Delta E = \frac{e^2}{2C} \tag{2}$$

where ΔE is the energy difference between the energy levels, but what is the meaning of the capacitance "C"? Equation (2) can not be true without a correct definition of the meaning of "C".

We will define *"C"* as *the capacitance between the maximum probability surfaces of finding the electron*.

To validate the suggested capacitance definition, we consider the Hydrogen atom and finding the capacitance between two '*s*' orbitals. Fig. (2) illustrates the maximum values of the probability of finding the electron $|\Psi|^2$ in '*s*' orbitals.

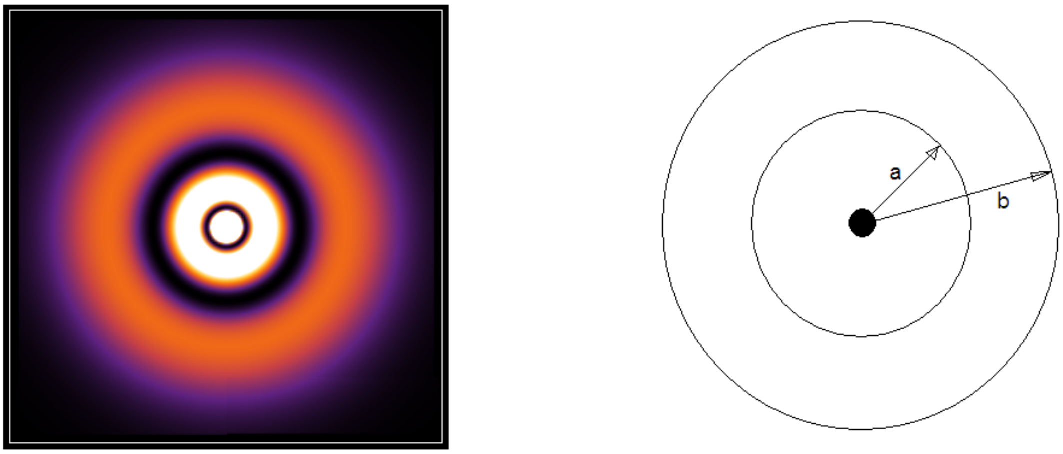

Fig. 2. The '*s*' orbitals of Hydrogen atom are represented as conducting spherical volumes and the maximum values of the probability of finding the electron (maximum of $|\Psi|^2$) are considered to be spheres with radiuses a, b, … .

The capacitance between two '*s*' orbitals according to our suggested definition is:

$$C = 4\pi\varepsilon_o \left(\frac{1}{a} - \frac{1}{b}\right)^{-1} \tag{3}$$

where ε_o is the permittivity of the vacuum, and a, b are the radiuses of the maximum probabilities spheres.

Substitute equation (3) in (1) and solve for $\frac{1}{\lambda}$:

$$\frac{1}{\lambda} = \frac{e^2}{8\pi\varepsilon_o hc}\left(\frac{1}{a} - \frac{1}{b}\right) \tag{4}$$

Equation (4) is the same as Bohr's formula for Hydrogen emission before applying the role of quantized angular momentum. This means that our definition of capacitance between quantum states works well.

An electrical model or equivalent circuit for atom's emission is the first application of the capacitance definition inside atom. In fig. 3, ΔE is replaced by its equivalent E_c. So for example, Hydrogen atom can be modeled by series of tunnel junctions as in Fig. (4).

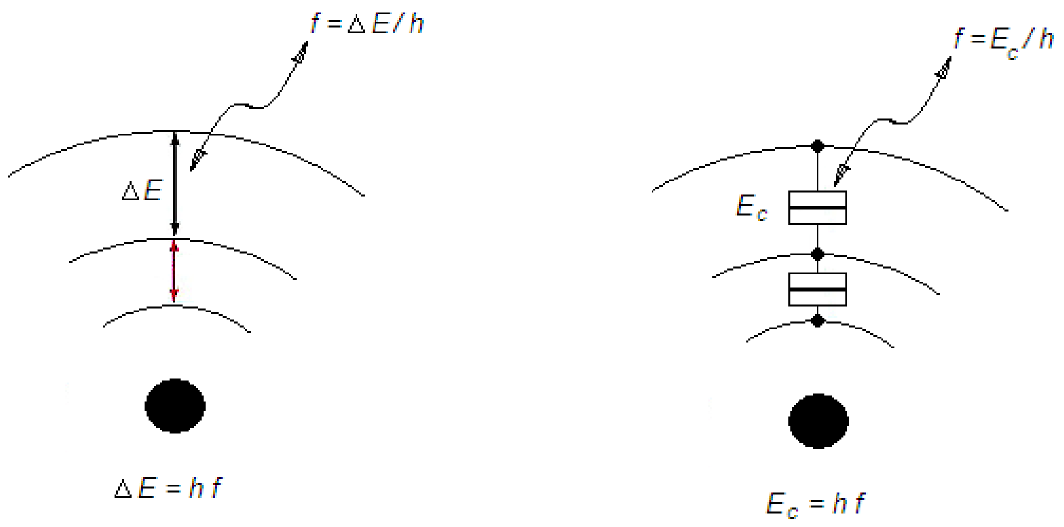

Fig. 3. ΔE is replaced by its equivalent E_c.

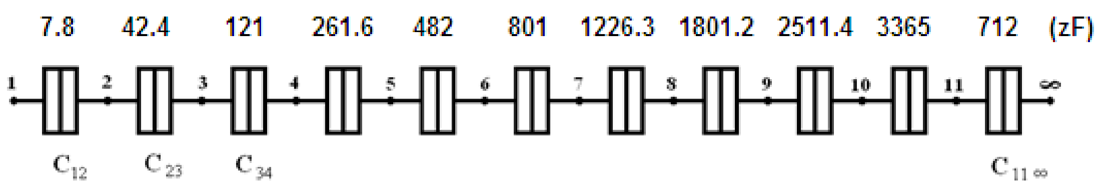

Fig. 4. Electrical model for Hydrogen Atom.

To validate capacitance definition for atoms which have more than one electron, the role of summing capacitors in series is used – see Figures 5 and 6. Fig. 7 represents a part of the equivalent circuit of Sodium and Iron atoms.

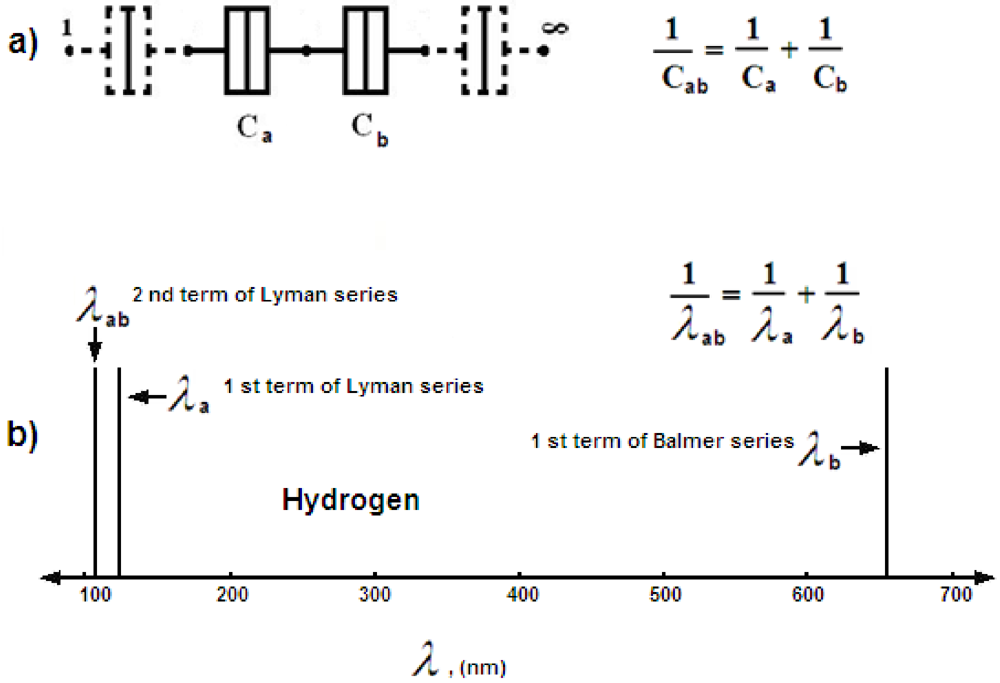

Fig. 5. The role of summing capacitors in series is also applied to the wave lengths of the line spectrum a) The role of summing capacitors in series, b) Example from the Hydrogen line spectrum.

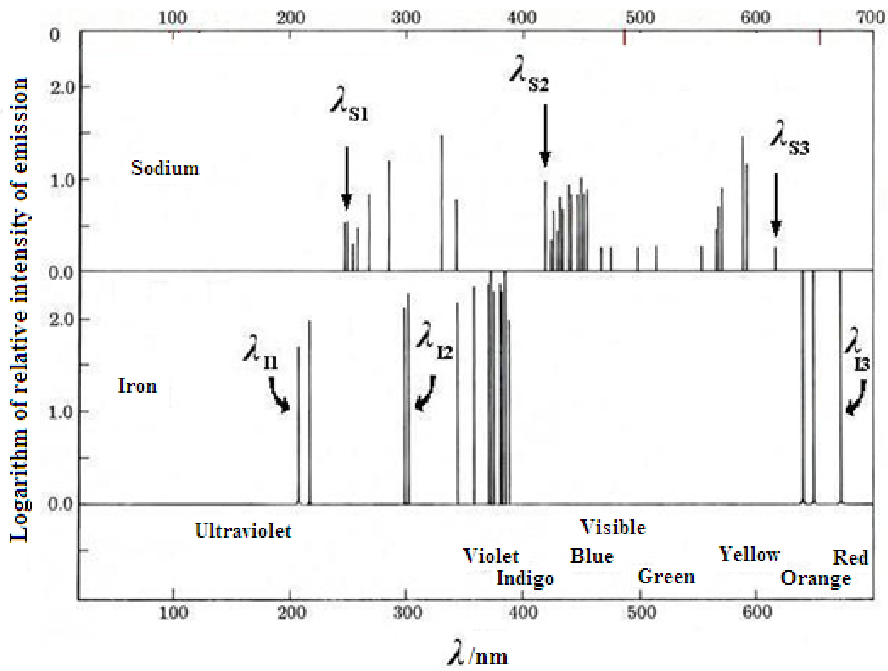

Fig. 6. Appling the role of summing capacitors in series on the spectra of Sodium and Iron. For Sodium $\frac{1}{\lambda_{S1}} = \frac{1}{\lambda_{S2}} + \frac{1}{\lambda_{S3}}$ **and for Iron** $\frac{1}{\lambda_{I1}} = \frac{1}{\lambda_{I2}} + \frac{1}{\lambda_{I3}}$ **(The spectrum without the arrows is from reference [3]).**

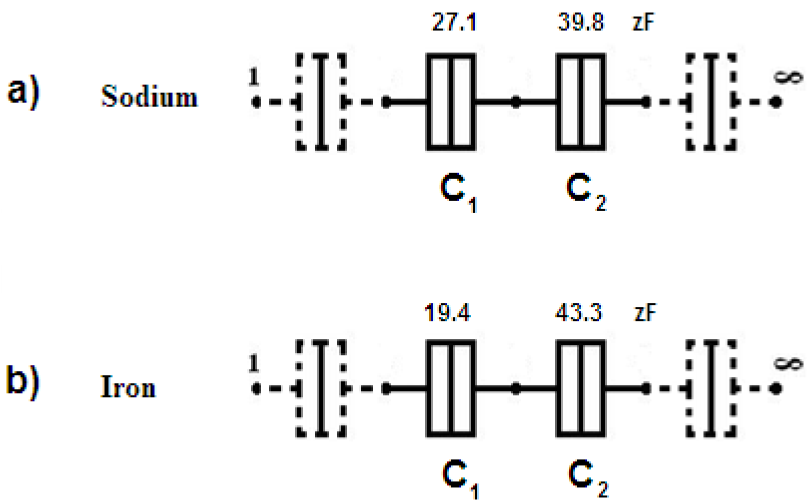

Fig. 7. Partial electrical models for a) Sodium and b) Iron atoms.

Another application of the concept of capacitance between orbitals is the analogy with the electronic band gap property. Band gap energy is a very important property for semiconductors and insulators. Also the capacitance between upper and lower quantum states of valence and conductance bands respectively can play the same role; further it has a more physical meaning than electronic band gap. Table (1) and Fig.(8) show the capacitance property for some materials.

It is probably better to say, *"The capacitance property of graphene is tunable by voltage drop"* than "*the electronic band gap is tunable by applied electric field*".

Table 1. Capacitance property of some semiconductor materials.

Material	Band Gap (eV)	Capacitance (zF)
AlN	6.2	12.9
GaN	3.4	23.53
SiC	3	27.67
InN	1.9	42.1
GaAs	1.4	57.14
Si	1.1	72.7
Ge	0.74	108.1
Starting of bilayer Graphene structure	0.25	320

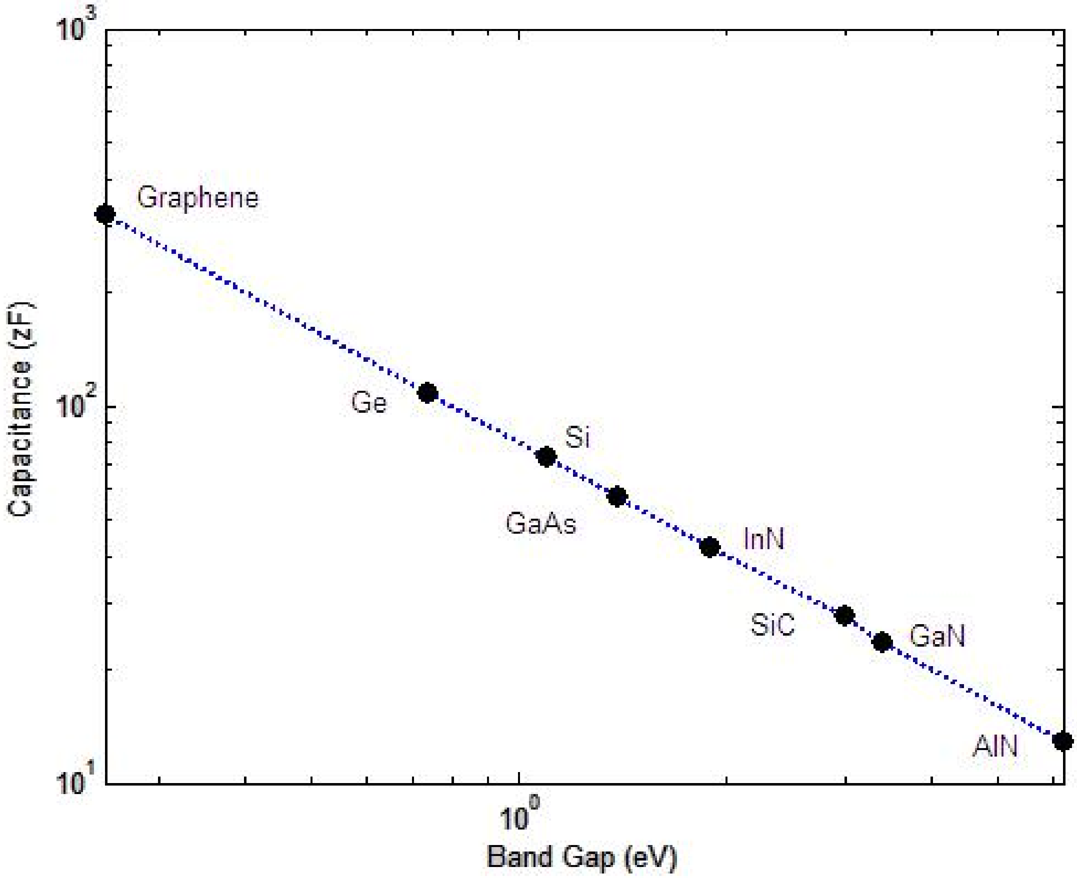

Fig. 8. Capacitance property against the band gap energy for materials listed in Table 1. Capacitance property is inversely proportional to the electronic band gap energy.

In this letter, the concept of capacitance between quantum states has been discussed. Electrical model for atoms is introduced (complete model for Hydrogen and partial models for Iron and Sodium). Finally the capacitance as a property of band gap materials is presented.

References:

1) Yuanbo Zhang et al: Nature **459**, 820 (2009).
2) K. K. Likharev and I. A. Devyatov: Physica B **194-196**, 1341 (1994).
3) http://chemed.chem.wisc.edu/chempaths/GenChem-Textbook/The-Visible-and-Ultraviolet-Spectra-of-Molecules-Molecular-Orbitals-1040.html (Access Date Sep. 10, 2013).