**Presentation title:** Harmonic and anharmonic lattice thermal capacity of nano-structured solids evaluated based on 3D GSM and q-deformed oscillator models

**Corresponding Author name:** Valeri LIGATCHEV

**Affiliation:** N/A

**Ph. No:** +65-91870780

**Email ID’s:** lva\_singapore@hotmail.com

**WhatsApp No:** +65-91870780

**Any alternative number:**

**Other Authors if any:** N/A

**Presentation type:** (Oral presentation/ Poster presentation)

**Abstract (250-300 words):**

Concept of so-called ‘*q*-numbers’, and closely related to it *q-deformed* oscillator attracted significant attention of researches in many areas of mathematics and physics since 1989. In particular, its well-known implementations comprise of analysis on the features of the *q-deformed* Harmonic Oscillator (Q-HO), and particularities of the *isobaric* temperature dependences of lattice thermal capacity, Cp(T), of bulk and nano-structured solids with the spatially ‘deformed’ atomic oscillations. Ii is noteworthy, that the Cp(T) quantity evaluated for solid semiconductors and insulators based on the Q-HO approach incorporates naturally both its *harmonic* and *anharmonic* fractions.

In this presentation, results of implementation of the Q-HO approach at evaluations on features of harmonic and anharmonic contributions to the Cp(T) function of nanostructured solids are discussed in comparison with predictions of the 3-dimensional (3D) Generalized Skettrup Model (GSM), which allows one to simulate realistically features of the Cp(T) function based on characteristics of the confined acoustic vibrations (phonons) with the static plane-wave basis. Both approaches yield readily the temperature dependencies for the harmonic and/or anharmonic fractions of Cp(T) dependence for 3D nano-structured solids, though implementation of the 3D GSM allows one to separate unambiguously contributions from its harmonic and anharmonic components as well as to take into account explicitly effect(s) of alteration(s) in sizes and dominant crystalline orientation of the nano-crystallites, while the Q-HO approximation provides rather formal interpretation for those energetic, thermal and morphological characteristics.

**Biography (150-200 words):**

Valeri Ligatchev’s areas of scientific interest and expertise comprise of experimental and computational studies on electronic, optical, vibrational, relaxation time and defect states spectra as well as thermal properties of various (predominantly spatially non-homogeneous) semiconductors insulators and even superconductors, including nominally undoped and heavily doped polycrystalline and nano-crystalline diamond(s), flakes of two-dimensional semiconductors, silicon-germanium ‘quantum dots’, ‘molecular wires’, silicon micro- and nano-wires, hydrogenated amorphous silicon-based films, porous ‘low-k’ organic and inorganic insulating layers, as well as ceramic insulators with ‘gigantic dielectric response’ (GDR).

His so-called ‘Generalized Skettrup Model’ becomes expedient in several important areas: from realistic simulations on optical and electronic properties of polycrystalline and spatially non-homogeneous amorphous semiconductors and insulators as well as of their low-dimensional counterparts to convincing estimations on the harmonic and anharmonic fractions of lattice thermal capacity of such materials; this model could be useful as well at quantitative evaluations on lifetimes of Fröhlich Polarons. He also substantiated condensed phases of Fröhlich polarons as the essence of the GDR phenomenon. Furthermore, he had implemented broadly advanced mathematical methods at deconvolution and interpretation of data of several well-established techniques of defect states spectroscopy.

Valeri Ligatchev is a member of The Electrochemical Society since 2007. His name had been included in 2011 Edition of Marquis Who's Who in the World.