

## Theoretical Chemistry Colloquium

**November 26, 2014 (Wed), 16:00-17:00**

**RCMS, 2<sup>nd</sup> floor, Chemistry Gallery**

### ***Influence of buffer gas and vibration temperature of carbon clusters on fullerene formation in a carbon plasma***

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**Abstract:** *A new method of calculation of fullerenes yield in carbon containing plasma is proposed. The method is based on the dynamic equations for the concentrations  $C(n, m, T, t)$ , where  $n$ -number of atoms in a carbon cluster,  $m$  is the number of the cluster dangling bonds,  $T$  is the temperature,  $t$ -current time. The method takes into account the electron concentration in the plasma and clusters heating/cooling during transformations when chemical bonds are formed or destructed. In addition, the clusters heating/cooling by a buffer gas influence is considered. The calculations give the qualitatively correct correlation between fullerenes yield in helium and argon buffer gas.*



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