# Physico-Chemical nanomaterials science

## Curvature and topological indexes for SiC nanoclusters

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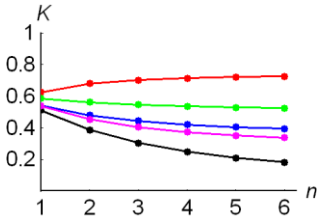
Topological (graph-theoretic) and related characterization tools are needed to understand fine structural peculiarities of very large scale clusters. Here we report some of our theoretical results in this field for SiC nanoclusters. For such nanoparticles it is especially important to grasp the structural differences of various SiC polytypes. To this end, we consider clusters of cubic (3C) and hexagonal (2*p*H, and $p \le 4$) polytypes with $10^4$ and more atoms. The Kirchhoff index (average resistance distance) surves us as a topological index. With this, we utilize the previously given electronic curvature *K* [1,2] as an electron-kinematic index. Specific computations show that, unexpectedly, topological indexes cannot well discriminate different polytypes. Unlike this, *K* make a clear discrimination between the polytypes. Namely, the following sequence is observed: $K[3C] < K[8H] < K[6H] < K[4H] < K[2H]$.




On the displayed plots of *K* vs. a conditional cluster length parameter *n*, we presented the results for 3C (black), 2H (red), 4H (green), 6H (blue), and 8H (magenta) polytypes. It is important that for these polytypes, the so-called hexagonality percentage shows the same ordering. The hexagonality measure long remained to be a lone index for distinguishing polytypes. Now we can add to it the electronic curvature as a useful electron-type measure.

1. *Luzanov A. V., Babich E. N.* Quantum-chemical quantification of molecular complexity and chirality // J Mol Struct (Theochem).-1995.-**333**, P. 279-290.
2. *Luzanov A. V., Nerukh D.* Complexity and chirality indices for molecular informatics: differential geometry approach // Funct Materials.-2005.-**12**, N 1.-P.55–64.