

研究论文

原子价壳层电子量子拓扑指数与元素电负性的关系

李忠海¹, 戴益民², 文松年², 聂长明^{*1,2}, 周丛艺²

(¹中南林学院生命科学与技术学院 长沙 410004)

(²南华大学化学化工学院 衡阳 421001)

收稿日期 2004-11-4 修回日期 2005-3-10 网络版发布日期 接受日期

摘要 在基态原子价壳层电子隐核图的基础上, 基于拓扑化学原理以及原子价壳层电子结构特征, 构建了原子价壳层电子量子拓扑指数(AEI), 它对基态原子实现唯一性表征, 结合原子价壳层电子平均化能($\sum n_i E_i / \sum n_i$)等参数, 建立了一套新的元素电负性标度: $X_N = -0.588710AEI_1 + 0.761214AEI_2 + 0.154982(\sum n_i E_i / \sum n_i) - 0.080929$. 该式给出了周期表中氢至镅共95种元素的电负性,

结果表明新电负性标度 X_N 与Pauling电负性标度颇为一致. 进一步从原子价轨道量子拓扑指数确定了sp, sp², sp³

杂化轨道的电负性. 新标度在元素和物质的结构-性质研究中具有一定的适用性.

关键词 [基态原子](#) [元素电负性](#) [价壳层电子](#) [量子拓扑指数](#) [轨道电负性](#)

分类号

Relationship between Atom Valence Shell Electron Quantum Topological Indices and Electronegativity of Elements

LI Zhong-Hai¹, DAI Yi-Min², WEN Song-Nian², NIE Chang-Ming^{*1,2}, ZHOU Cong-Yi²

(¹ School of Life Science and Technology, Central South Forestry University, Changsha 410004)

(² School of Chemistry and Chemical Engineering, Nanhua University, Hengyang 421001)

Abstract A novel atom valence shell electron quantum topological index AEI based on topological chemical principle and atom valence shell electron structure character with the help of hidden core graph of ground state atom valence shell electron was proposed in this paper, which appears uniquely to the ground state atom and has excellent structural selectivity. With combining even ionization energy of atom valence shell electrons ($\sum n_i E_i / \sum n_i$), a new elemental

electronegativity scale X_N was put forward: $X_N = -0.588710AEI_1 + 0.761214AEI_2 + 0.154982(\sum n_i E_i / \sum n_i) - 0.080929$.

By the formula the electronegativities of 95 elements from hydrogen to americium have been obtained. The results indicate that the new electronegativity scale X_N was in conformity very well with Pauling scale. Moreover, orbital

electronegativities of sp, sp², sp³ for carbon atom can be obtained from atom valence orbital quantum topological index using the same method. The new electronegativity scale of elements can be widely applied to the study of structure-property relationship of elements and materials.

Key words [ground state atom](#) [electronegativity of element](#) [valence shell electron](#) [quantum topological index](#) [orbital electronegativity](#)

DOI:

通讯作者 聂长明 niecm196132@163.com

扩展功能

本文信息

▶ [Supporting info](#)

▶ [PDF\(469KB\)](#)

▶ [\[HTML全文\]\(0KB\)](#)

▶ [参考文献](#)

服务与反馈

▶ [把本文推荐给朋友](#)

▶ [加入我的书架](#)

▶ [加入引用管理器](#)

▶ [复制索引](#)

▶ [Email Alert](#)

▶ [文章反馈](#)

▶ [浏览反馈信息](#)

相关信息

▶ [本刊中 包含“基态原子”的 相关文章](#)

▶ 本文作者相关文章

- [李忠海](#)
- [戴益民](#)
- [文松年](#)
- [聂长明](#)
- [周丛艺](#)