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ABSTRACT SYMPOSIUM NAME: Southwest Theoretical & Computational Chemistry (Invited) (Oral)
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TITLE: Topological properties for some cubic crystallographic lattice clusters
ABSTRACT BODY:
Abstract: We investigate face centered and body centered cubic clusters as a function of the number of vertices, N, and number of cluster shells, L. The number of links, vertices, coordination numbers and exterior vertices exhibit ‘magic number’ characteristics versus L, as the size of the clusters increases. Starting with only the spatial coordinates, we create an adjacency and distance matrix that facilitates the calculation of topological indices, including the Wiener, hyper-Wiener, reverse Wiener, Szeged, Balaban, and Kirchhoff indices. Some known topological formulas for some platonic solids when L = 1 are computationally verified. The asymptotic limits with N of the topological indices are shown to exhibit power law behavior whose exponent depends on the dimension of 3D space and type of topological index. The asymptotic graph energy and the Laplacian energy is linear with N. Also, the Shannon entropy of these lattices shows logarithmic behavior with increasing N.

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