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Title

Chemistry: The coupling science

Authors

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Abstract

We make the case for an enhanced adoption of matrix algebra in undergraduate chemical curriculum by laying out an example-driven perspective of Chemistry as a discipline that focuses on interactions—couplings—among various microscopic entities.

Many Physical Chemistry textbooks and courses emphasize an operator-driven approach to Quantum Chemistry, favoring it over the equivalent matrix formalism. For example, one particularly popular textbook, does not even mention matrices until the discussion of the Hückel molecular-orbital theory (MO).

We argue that educators' adherence to the operator-only approach misses a pedagogical opportunity to help create a highly beneficial parallel framework of Chemistry in learners' minds. This missing framework would conceptualize *early on* that Chemistry is not something that happens to stand-alone electrons, atoms, or molecules. Instead, Chemistry is all about interactions.

The easiest—and most intuitive—way to describe many types of interactions mathematically is by using matrices. Many students and educators shy away from them, but matrices can be easily and intuitively understood as simply interaction or coupling tables. To a beginning learner's brain, the idea of a *table* is much less abstract than that of an *operator*. Yet tables (i.e., matrices) can be used as simple tools for building powerful conceptual frameworks for describing chemical forces using fairly simple *algebra* instead of differential and integral *calculus* inherent in the operator representation.

We will discuss several well- and less-well-known applications of matrices in chemistry, including a Fourier view of quantum confinement, vibrational mode couplings, and MO theory. In particular, we will describe a new density-matrix adaptation of the Hückel MO theory to general bonding scenarios in which the original Hückel model simply does not apply.

Track

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28th Feb 2024, 6:03pm EST

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