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Spectral theory for molecules and materials: Pauli revisited PETER W. LANGHOFF, SDSC/UCSD, MICHAL BEN-NUN, UCSD, JEFFREY MILLS, JERRY BOATZ, AFRL/RZSP — Implementations of new theoretical methods are reported for *ab initio* chemical structure calculations of molecules and materials based on an atomic spectral-product representation of aggregate electronic degrees of freedom. In this approach, the Pauli principle is enforced subsequent to construction of the Hamiltonian representative matrix in the basis, greatly simplifying its evaluation. It is shown that atomic pair-interaction calculations, which can be performed once and for all and retained for repeated applications, are sufficient to determine the electronic eigenstates and chemical structures of arbitrary chemical aggregates. The spectral-product representation is seen to span the totally antisymmetric representation of the aggregate electron symmetric group once and only once, but to also span other non-Pauli representations in which the desired Pauli solutions of the Schrödinger equation are generally embedded. Progress in isolating totally antisymmetric solutions is described employing the antisymmetrizer matrix constructed in the spectral-product basis. The Pauli subspace of the full spectral-product Hilbert space is isolated in this manner, and the corresponding physical block of the aggregate Hamiltonian matrix determined. Illustrative calculations of ground- and excited-state potential energy surfaces in simple molecules exhibit convergence to corresponding totally antisymmetric results.

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