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The Role of Quantum Stress in Descriptive Chemistry[1] ILYA TOKATLY[2], Lehrstuhl für Theoretische Festkörperphysik, Universit"at Erlangen-Nürnberg, Germany, GIOVANNI VIGNALE, University of Missouri-Columbia, JIANMIN TAO, Los Alamos National Laboratory — We show that key concepts of descriptive chemistry, such as atomic shells, bonding electron pairs and lone electron pairs, may be described in terms of *quantum stress focusing*, i.e. the spontaneous formation of closed surfaces upon which the electronic pressure has an extremum. This description subsumes previous mathematical constructs, such as the Laplacian of the density and the electron localization function, and provides a new tool for visualizing chemical structure. We also show that the full anisotropic stress tensor can be easily calculated from density functional theory.

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