

## Activation of polar bonds by electric fields: An Electron Localization Perspective

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**Abstract:** The electron localization induced by an external electric field is evaluated using the information content of the same-spin conditional pair density [1]. In this work we consider the stretching of the C-X (X: halogen) bonds of methyl halide molecules, under the experience of a homogeneous static electric field and a static heterogeneous one, created by a source of point charges. In addition, in order to assess the importance of ionic structures throughout the chemical bond breaking, we project the Generalize Valence Bond (GVB) wave-function in their classical covalent and ionic structures (see for instance [2]). The increase of electric fields, is expected to have a reorganization of the electrons when the bond is subjected under a strong enough field. These general observations are thoroughly explained using a simple Valence Bond model that involve the increment of the resonance energy between the covalent and the ionic structures and the curve crossing between the two structures after some field strength.

**Key-words**: Valence Bond Theory, External Electric Fields, Electron Localization, Methyl Halide Bonds.

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