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Electric Field-enhanced Intermolecular Bonding: an Ab Initio Density Functional Investigation RAJEEV PATHAK, University of Pune, MH, India — Effects of external electric field on some otherwise weakly bound molecular complexes are investigated within the density functional theory. The complexes are comprised of polar and non-polar molecules, which otherwise interact via van der Waals bond, or through a weak hydrogen bond. Applied field distorts the geometry and forces the molecules to come closer to each other leading to a remarkable enhancement in the bonding between the otherwise weakly bonded atoms. We investigate this phenomenon with the density functional theory applied two prototype systems in external electric field, viz. acetylene + water and carbon-dioxide + water systems where the applied field strengthens the bonding, considerably so in the latter case.

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