Molecular electronic excitations and the minimum polarizability principle

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The validity of the minimum polarizability principle upon electronic excitation is studied as a companion principle of that obtained by Chattaraj and Poddar in the case of the maximum hardness principle. Twelve diatomic molecules have been selected and, both the hardness and the dipole polarizability for the ground and excited states have been calculated by means of ab initio density functional calculations using Sadlej's basis set. It has been found that a molecule is less polarizable in its ground state than in an electronically excited state of the same spin multiplicity.