Quantum Chemical Analysis of the Dielectric Constant Concept at Atomic Scale: an Interaction of Probing Point Charges with Silica Cristobalite-Like Cluster

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The quantum chemically simulated interaction of probing point charges with the silica cristobalite-like cluster $Si_{48}O_{122}H_{52}$ [= $Si_{48}O_{70}(OH)_{52}$] proves that the macroscopic dielectric constant can not be used at atomic scale distances due to quantum chemical interactions.

Key words: Dielectric Constant; Quantum Chemistry; Semi-Empirical Method; PM3; Silica.