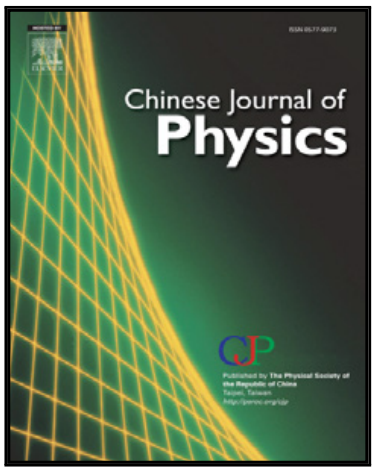

A density functional theory study of double proton transfer reactions in formamide, formamide-formic acid and formic acid dimers

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Highlights

- A detailed reaction mechanism for the double proton transfers in formamide and formic acid dimers is revealed..
- The reaction forces, the chemical potentials and the reaction electronic fluxes are presented.
- The SAPT energy decomposition analysis reveals the dominant exchange energy contribution to the reaction barriers.