Can an entirely negative fluorine in a molecule, viz. perfluorobenzene, interact attractively with the entirely negative site(s) on another molecule(s)? Like liking like!

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Supplementary Information

Fig. S1: RDG vs. Sign(λ_2)×ρ (left) and RDG = 0.6 a.u. isosurface (right) NCI graphical plots for $H_3N\cdots FC_6F_5$. The spikes in the $\lambda_2 < 0$ and $\lambda_2 > 0$ regions represent to the bonded (attractive) and non-bonded (repulsive) interactions, respecctively. The respective s = 0.6 a.u. RDG isosurfaces painted in green and red are depicted in Fig. 2 (see the ball and stick models). (Also, see Fig. 1 for conformational details, and that the dimer labeling in Fig. 1 is in consistent with that shown in Fig. 2 for QTAIM and RDG based molecular and RDG plots, respectively).

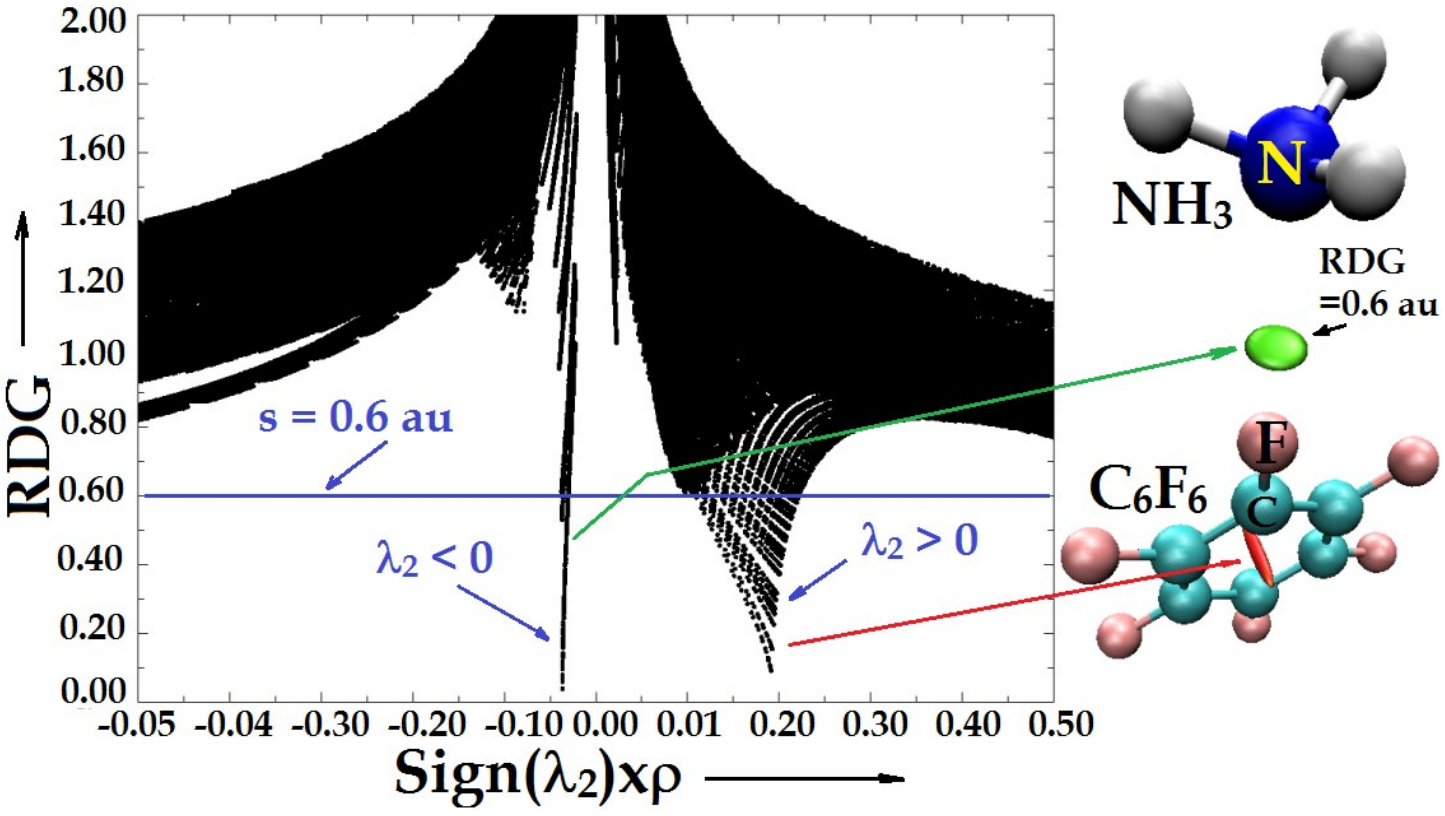

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Fig. S2: RDG vs. Sign(λ_2)×ρ plot for $H_2O\cdots FC_6F_5$ a), $H_2O\cdots FC_6F_5$ b), $H_3CF\cdots FC_6F_5$ c), $H_3CF\cdots FC_6F_5$ d), $HF\cdots FC_6F_5$ e) and $HF\cdots FC_6F_5$ f) (values in a.u.). The spikes in the $\lambda_2 < 0$ and $\lambda_2 > 0$ regions represent to the bonded (attractive) and non-bonded (repulsive) interactions, respecctively. The respective s = 0.6 a.u. RDG isosurfaces painted in green and red are depicted in Fig. 2 (see the ball and stick models). (Also, see Fig. 1 for conformational details, and that the dimer lableing in Fig. 1 is in consistent with that shown in Fig. 2 for QTAIM and RDG based molecular and RDG plots, respectively).

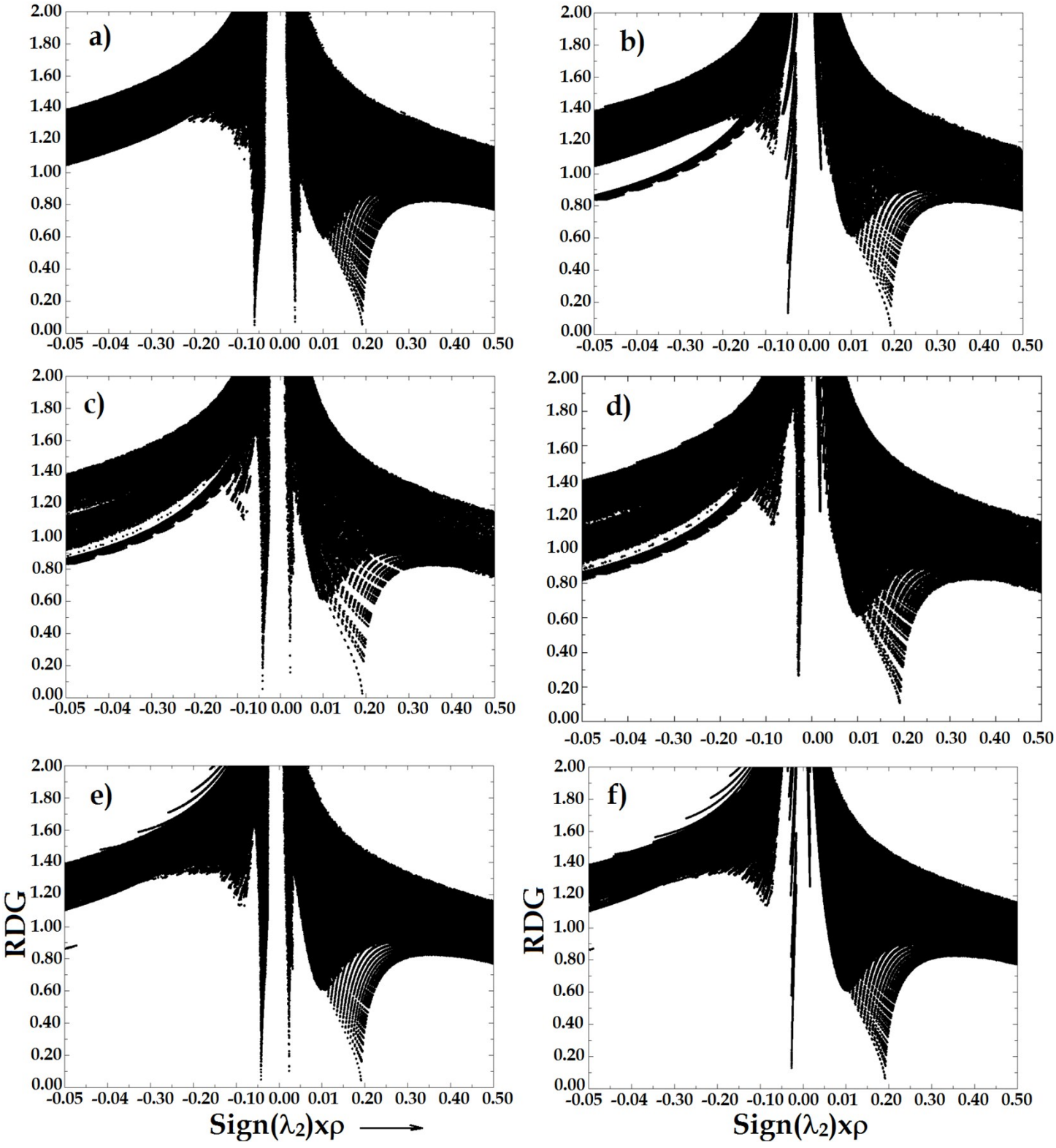

Fig. S3: RDG vs. Sign(λ_2)×ρ plot for $H_2CO\cdots FC_6F_5$ h), $H_2CO\cdots FC_6F_5$ i), $C_5F_5N\cdots FC_6F_5$ j), $C_4F_4N_2\cdots FC_6F_5$ k), $C_4F_4N_2\cdots FC_6F_5$ l), and $(CF)_4N_2\cdots FC_6F_5$ m) (values in a.u.). The spikes in the $\lambda_2 < 0$ and $\lambda_2 > 0$ regions represent to the bonded (attractive) and non-bonded (repulsive) interactions, respecctively. The respective s = 0.6 a.u. RDG isosurfaces painted in green and red are depicted in Fig. 2 (see the ball and stick models). (Also, see Fig. 1 for conformational details, and that the dimer lableing in Fig. 1 is in consistent with that shown in Fig. 2 for QTAIM and RDG based molecular and RDG plots, respectively).