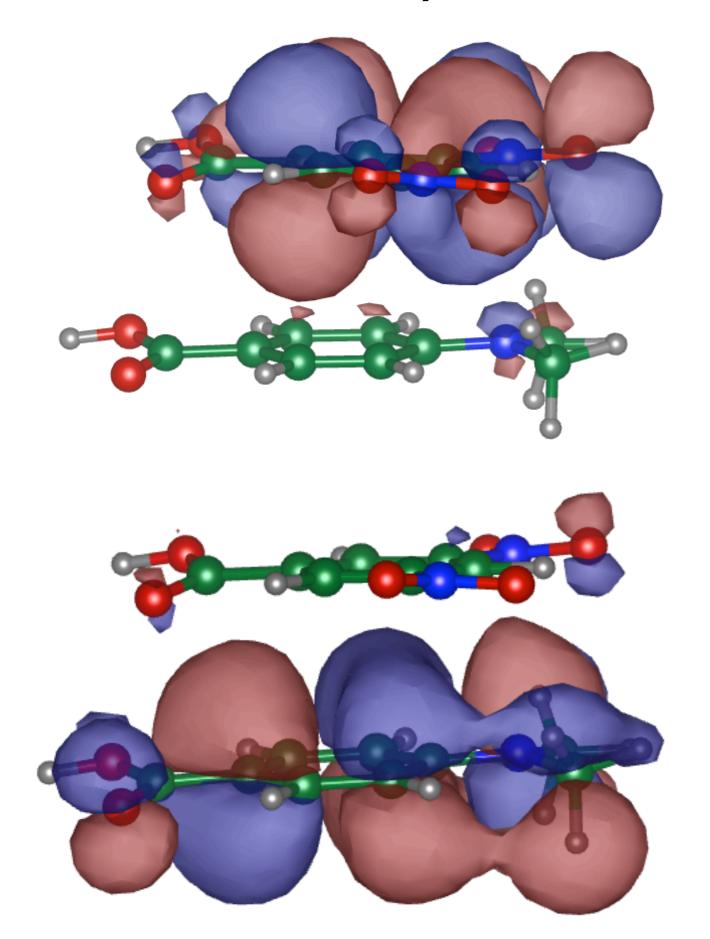
Electronic Supplementary Material (ESI) for CrystEngComm This journal is © The Royal Society of Chemistry 2012

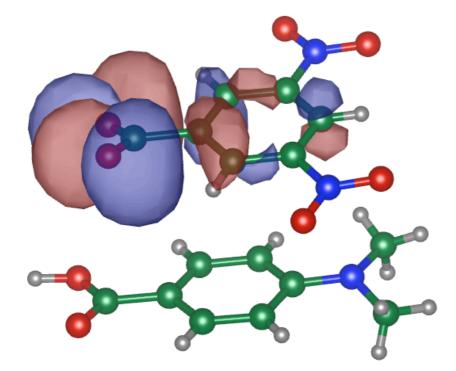




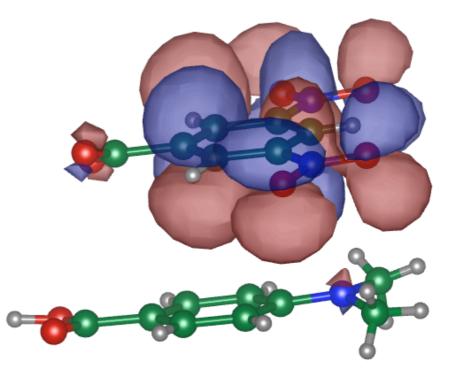
LUMO of 3,5-dnba/ 4-dmaba dimer E = -1.9118 eV

HOMO of 3,5-dnba/ 4-dmaba dimer E =-7.056 eV Electronic Supplementary Material (ESI) for CrystEngComm This journal is © The Royal Society of Chemistry 2012

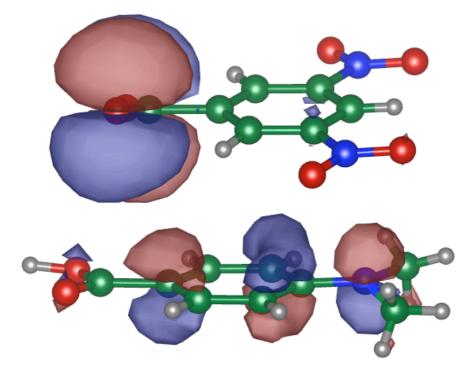




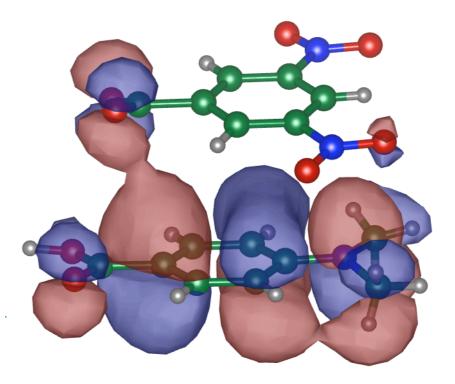
LUMO of 3,5-dnba<sup>-</sup>/4-dmaba dimer E = 1.1755 eV



HOMO of 3,5-dnba<sup>-</sup>/4-dmaba dimer E = -3.9981 eV

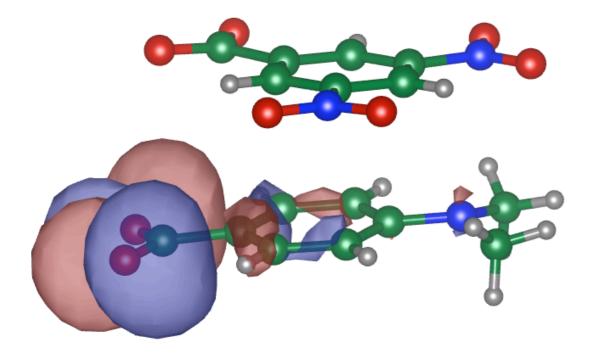


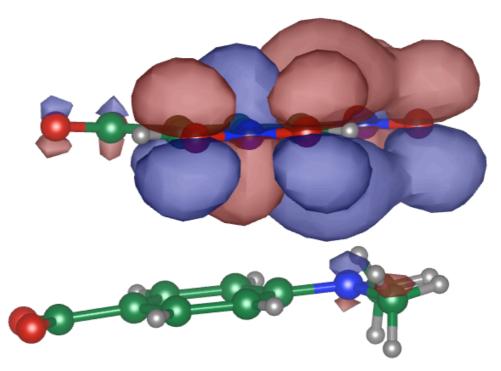
 $2^{nd}$  HOMO of 3,5-dnba<sup>-</sup>/4-dmaba dimer E = -4.0582 eV



 $3^{rd}$  HOMO of 3,5-dnba<sup>-</sup>/4-dmaba dimer E = -4.1625 eV Electronic Supplementary Material (ESI) for CrystEngComm This journal is © The Royal Society of Chemistry 2012

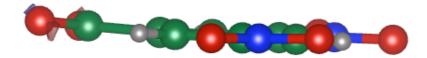


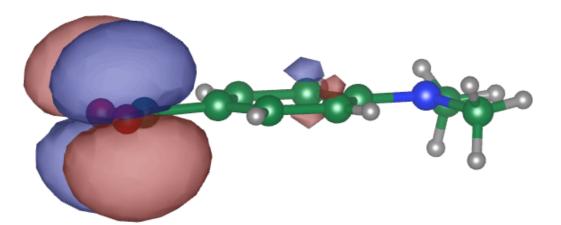




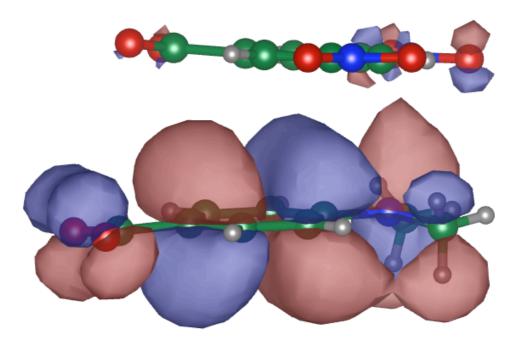
LUMO of 3,5-dnba<sup>-</sup>/4-dmaba<sup>-</sup> dimer E = 3.5366 eV

HOMO of 3,5-dnba<sup>-</sup>/4-dmaba<sup>-</sup> dimer E = -0.1239 eV





 $2^{nd}$  HOMO of 3,5-dnba<sup>-</sup>/4-dmaba<sup>-</sup> dimer E = -0.246 eV



 $3^{rd}$  HOMO of 3,5-dnba<sup>-</sup>/4-dmaba<sup>-</sup> dimer E = -0.6176 eV