

DFT computational study of trihalogenated aniline derivative's adsorption onto nanocages
Jamelah S.Al-Otaibi^a, Y.Sheena Mary^{b*}, Y.Shyma Mary^b, Savaş Kaya^c, Goncagül Serdaroglu^d

^a Department of Chemistry, College of Science, Princess Nourah bint Abdulrahman University, Saudi Arabia

^b Researcher, Thushara, Neethinagar-64, Kollam, Kerala, India

^c Sivas Cumhuriyet University, Health Services Vocational School, Department of Pharmacy, 58140, Sivas, Turkey

^d Sivas Cumhuriyet University, Faculty of Education, Math. and Sci. Edu., 58140 Sivas/ TURKEY

*Author for correspondence: email: marysheena2018@rediffmail.com

Fig.S1.1. DOS plot of FA

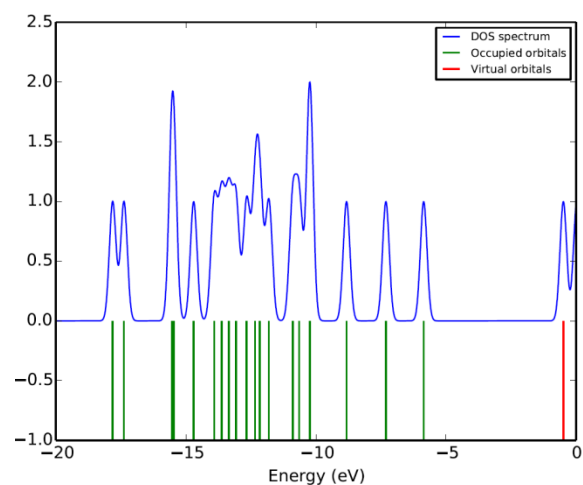


Fig.S1.2 DOS plots of G-FA and F-FA

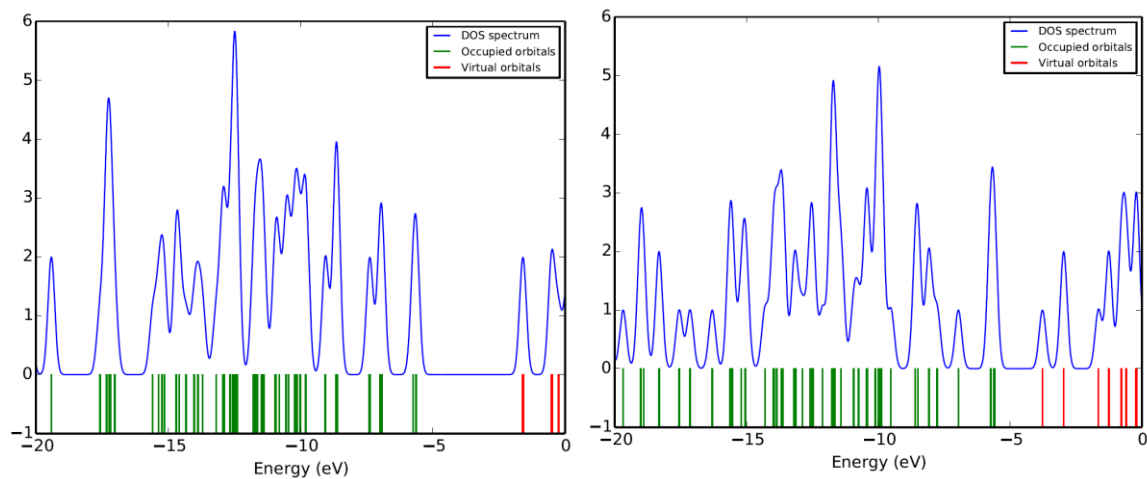


Fig.S1.3 DOS plots of AlN-FA and AIP-FA

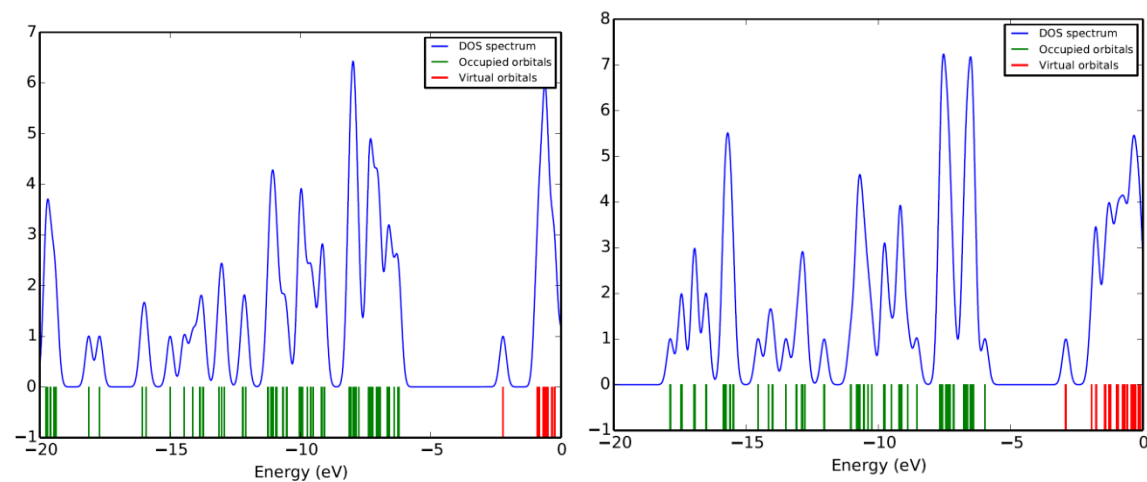


Fig.S1.4 DOS plots of BN-FA and BP-FA

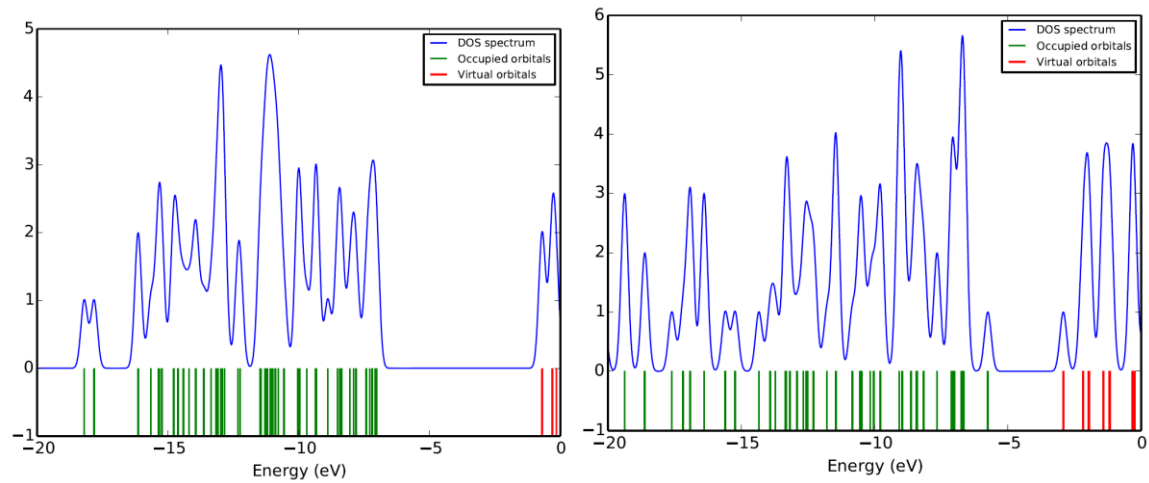


Fig.S1.5 DOS plot of CA

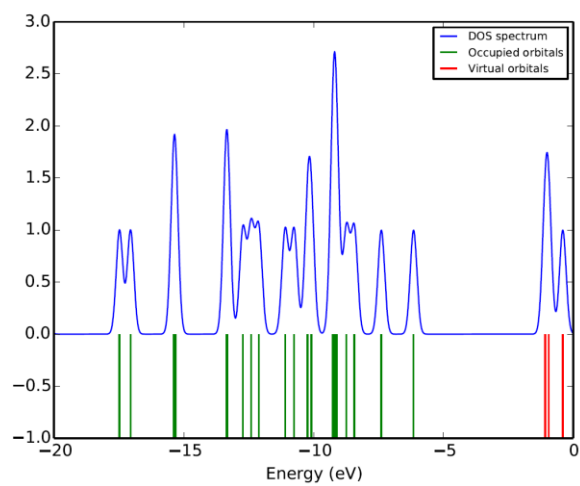


Fig.S1.6 DOS plots of G-CA and F-CA

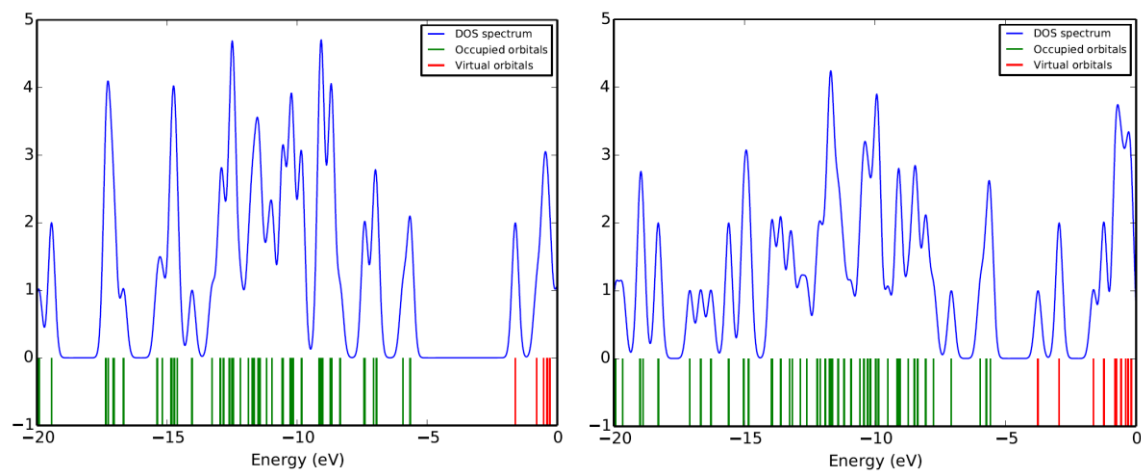


Fig.S1.7 DOS plots of AlN-CA and AlP-CA

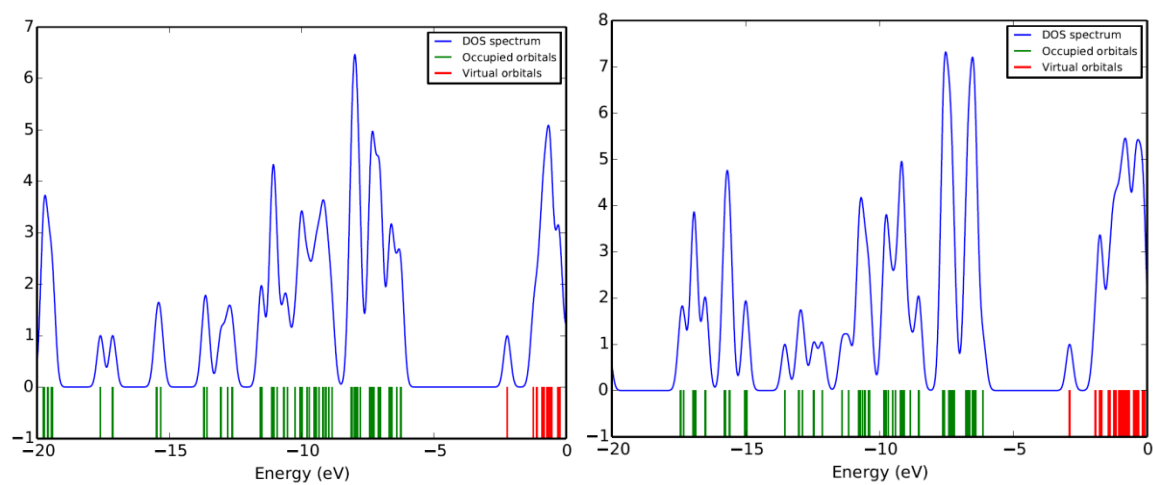


Fig.S1.8 DOS plots of BN-CA and BP-CA

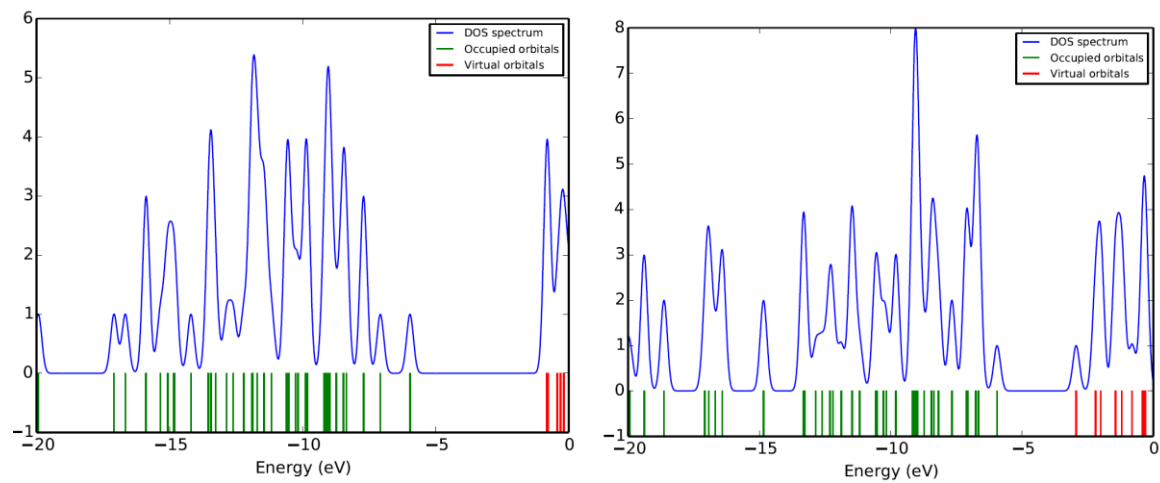


Fig.S1.9 DOS plot of BA

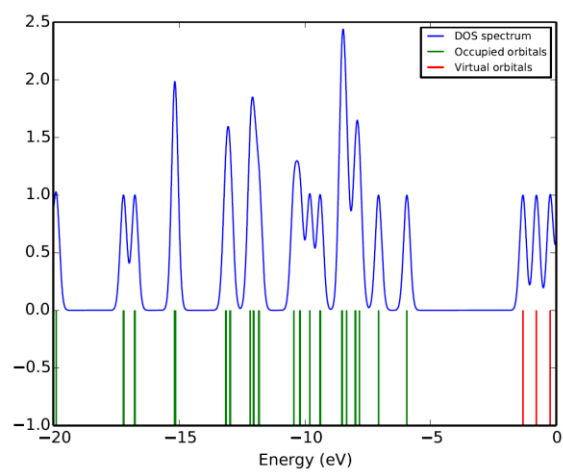


Fig.S1.10 DOS plots of G-BA and F-BA

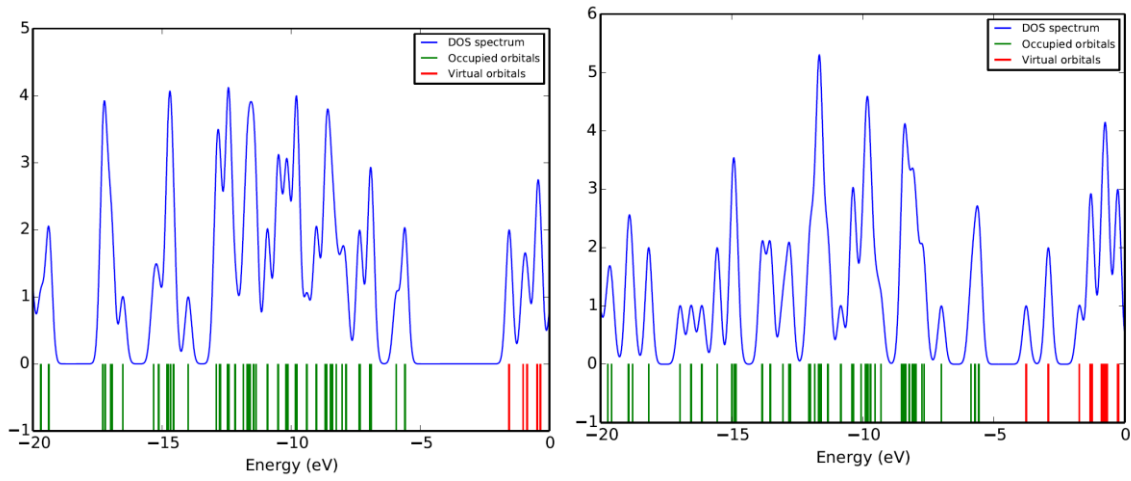


Fig.S1.11 DOS plots of AlN-BA and AlP-BA

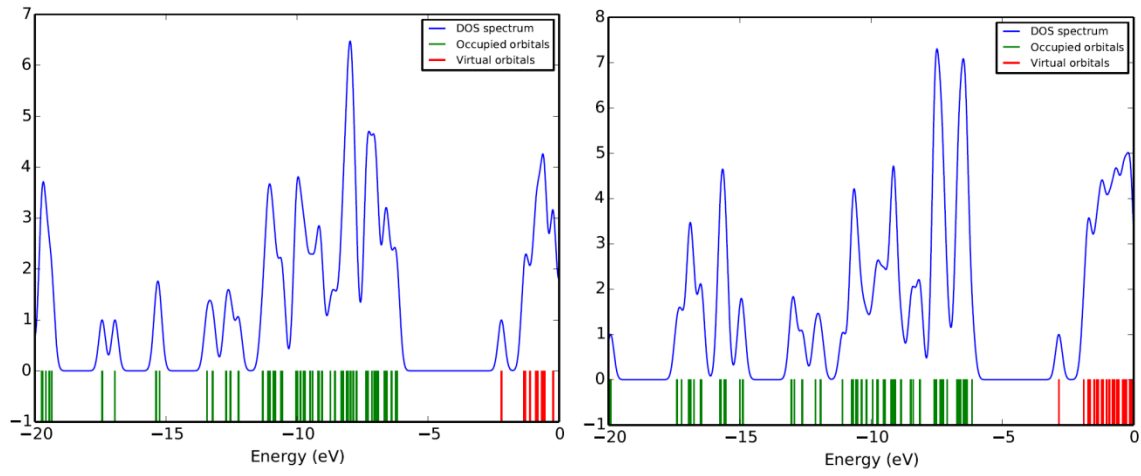


Fig.S1.12 DOS plots of BN-BA and BP-BA

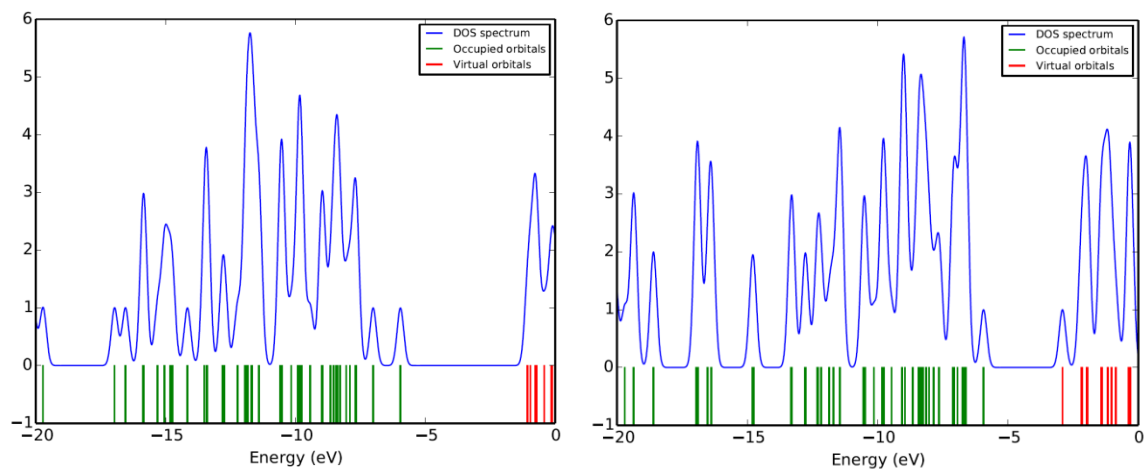


Fig.S2.1 UV spectrum of FA

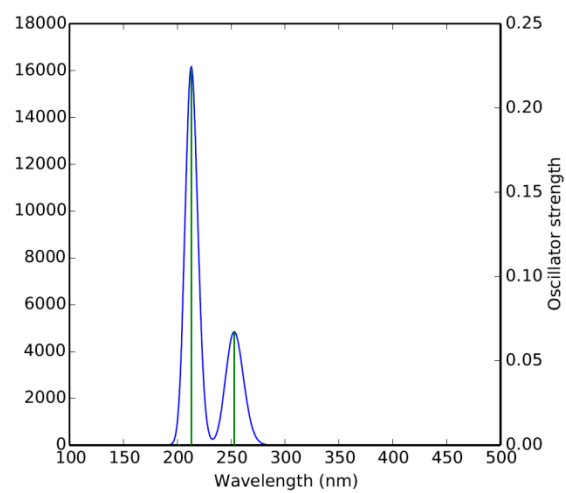


Fig.S2.2 UV spectrum of G-FA and F-FA

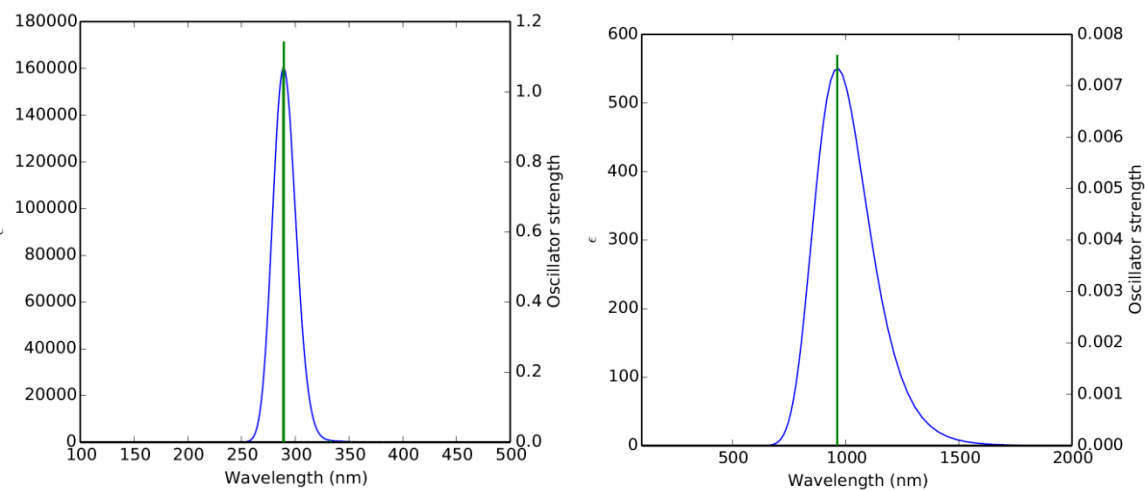


Fig.S2.3 UV spectrum of AlN-FA and AlP-FA

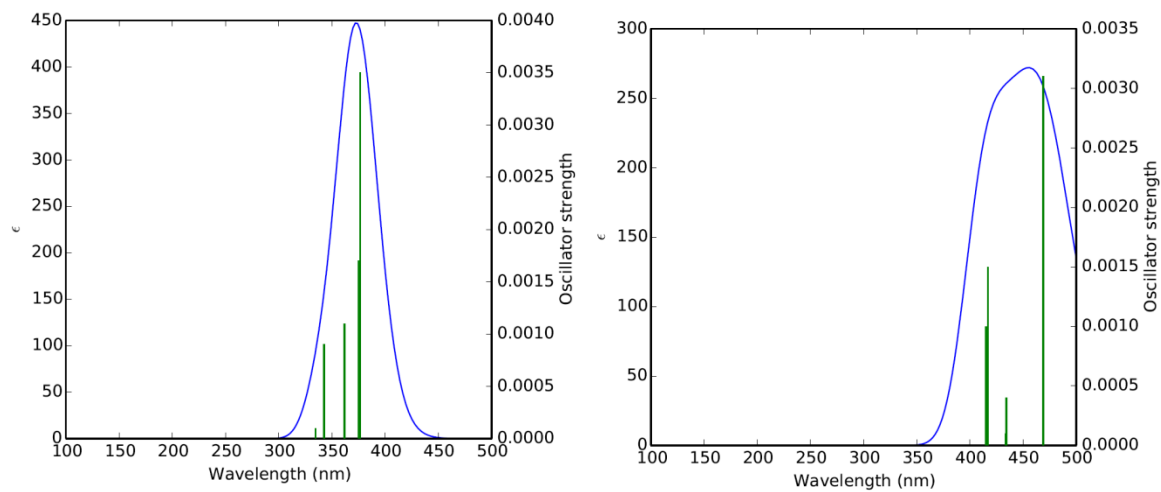


Fig.S2.4 UV spectrum of BN-FA and BP-FA

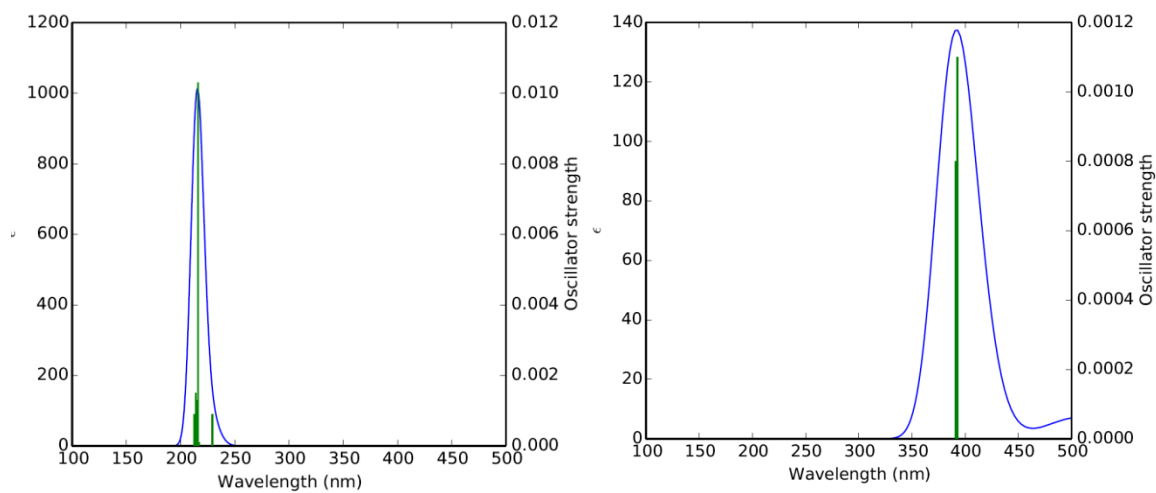


Fig.S2.5 UV spectrum of CA

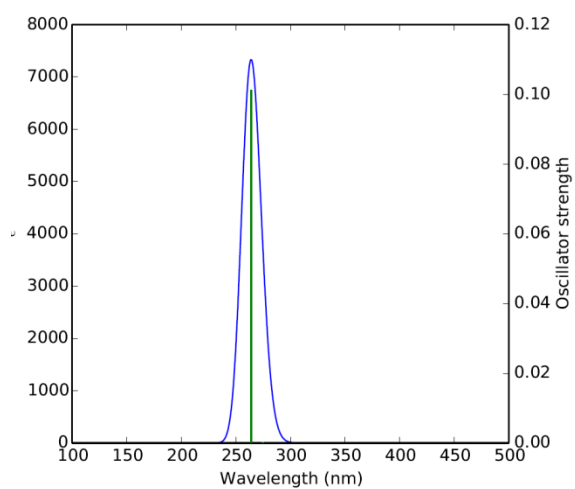


Fig.S2.6 UV spectrum of G-CA and F-CA

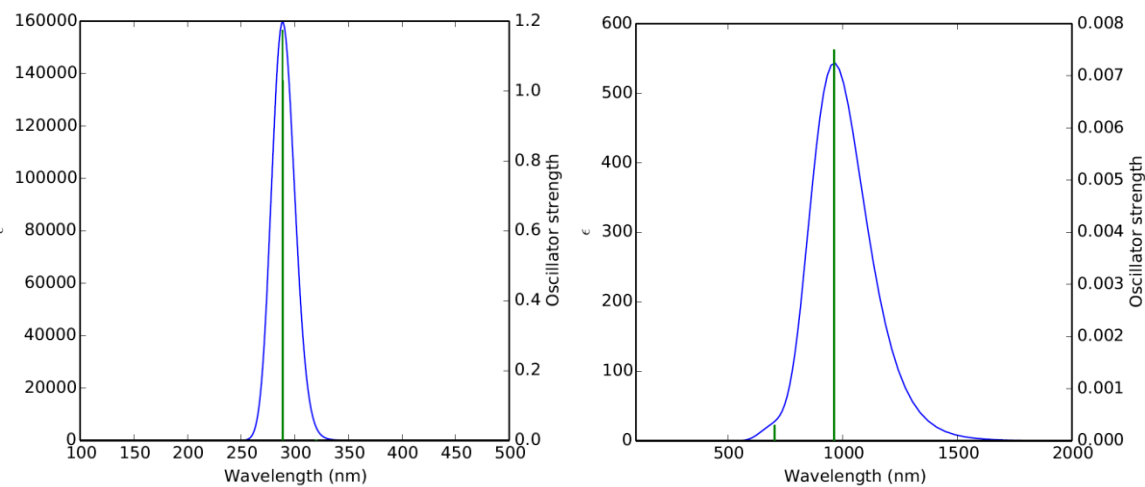


Fig.S2.7 UV spectrum of AlN-CA and AlP-CA

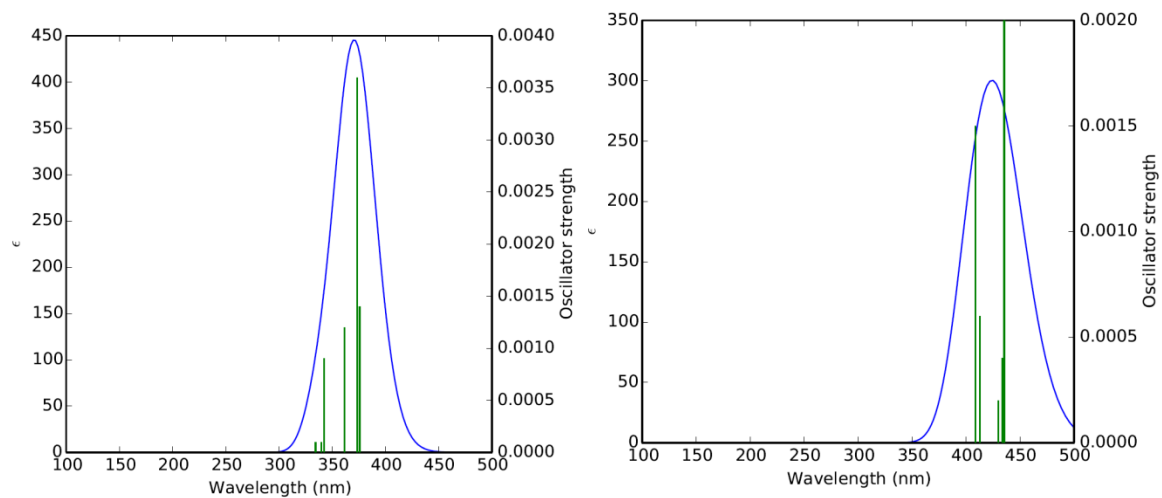


Fig.S2.8 UV spectrum of BN-CA and BP-CA

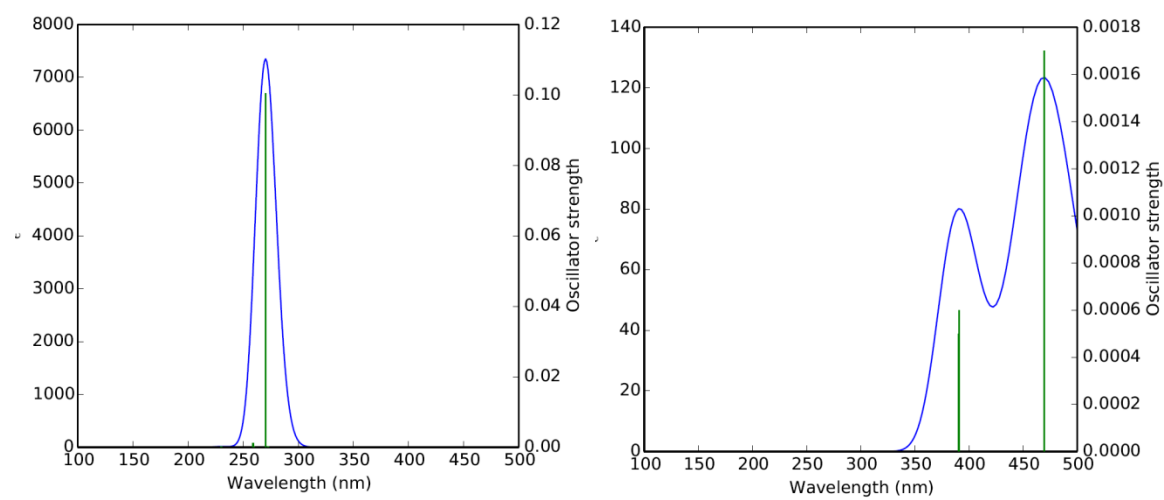


Fig.S2.9 UV spectrum of BA

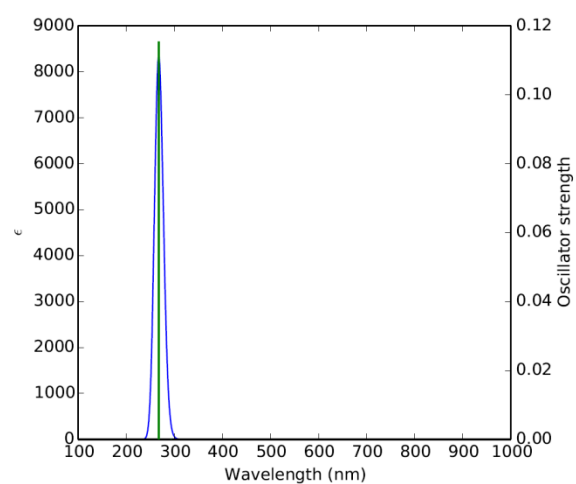


Fig.S2.10 UV spectrum of G-BA and F-BA

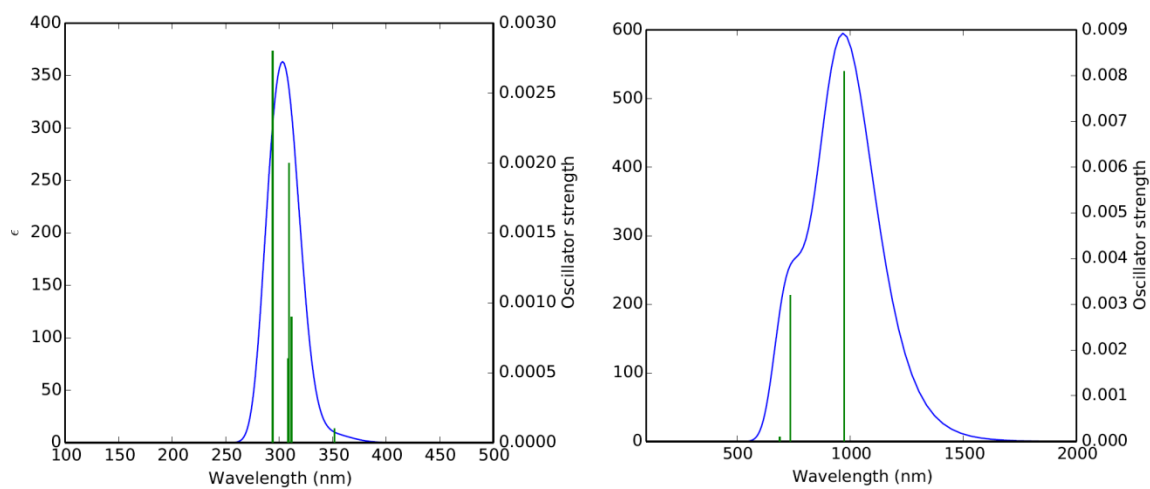


Fig.S2.11 UV spectrum of AlN-BA and AlP-BA

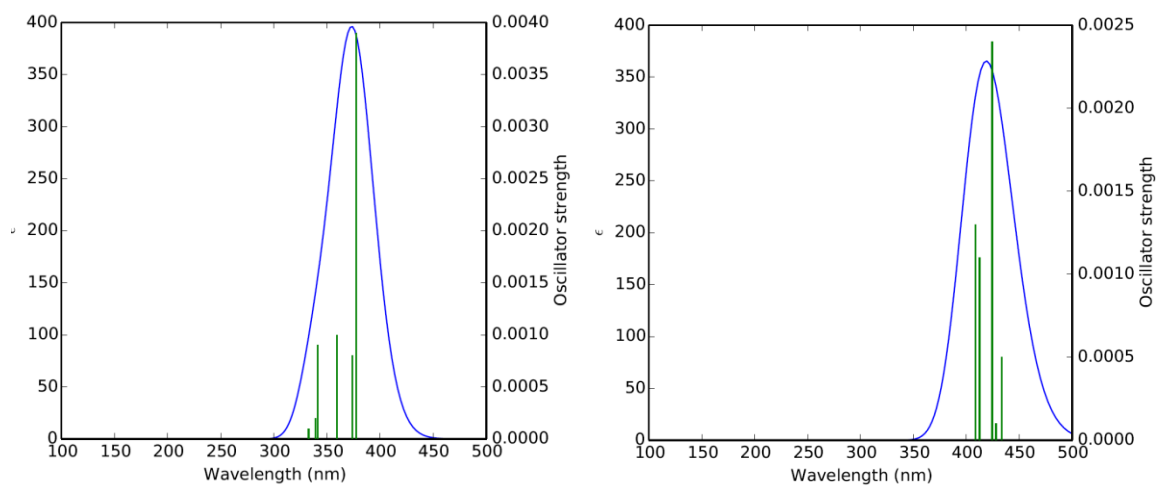


Fig.S2.12 UV spectrum of BN-BA and BP-BA

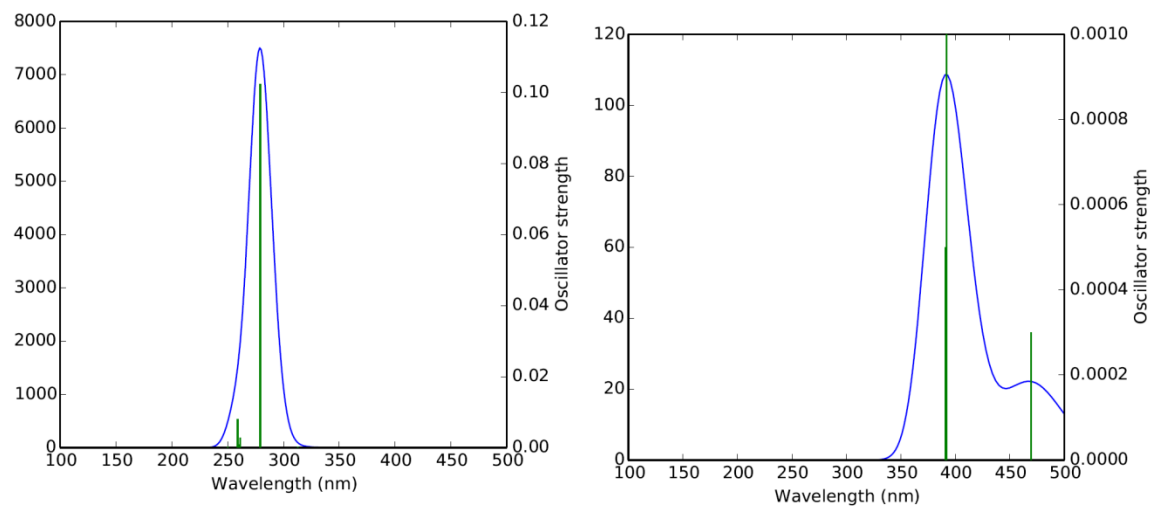


Fig.S3 Raman spectrum (DFT) of (a) FA (b) CA (c) BA

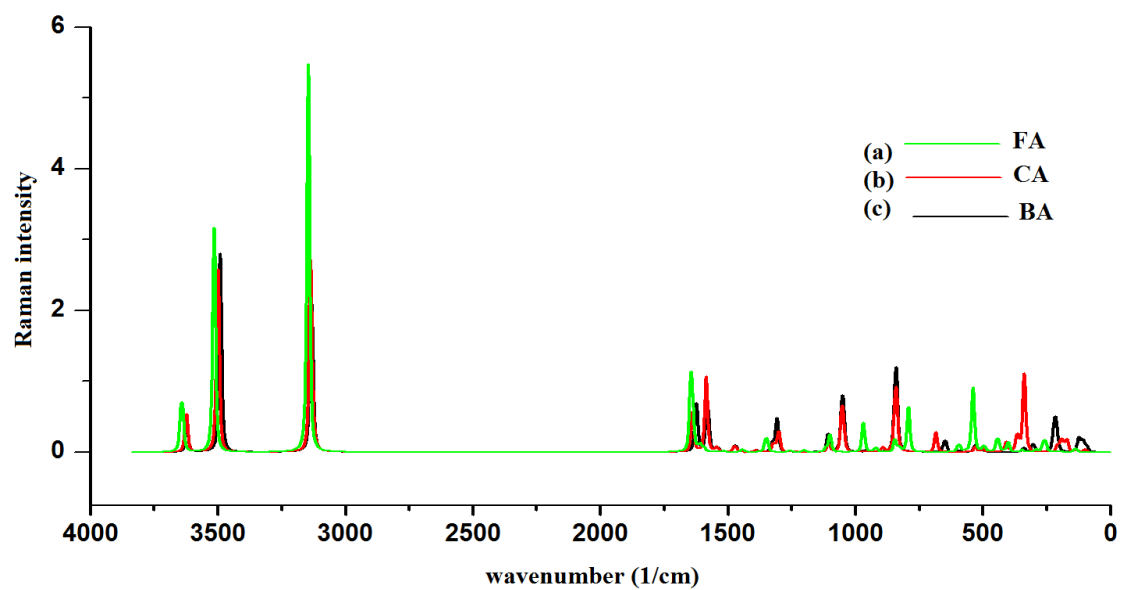


Fig.S4.1 Raman spectrum of (a) G-FA (b) F-FA (c) AlN-FA (d) AlP-FA (e) BN-FA (f) BP-FA

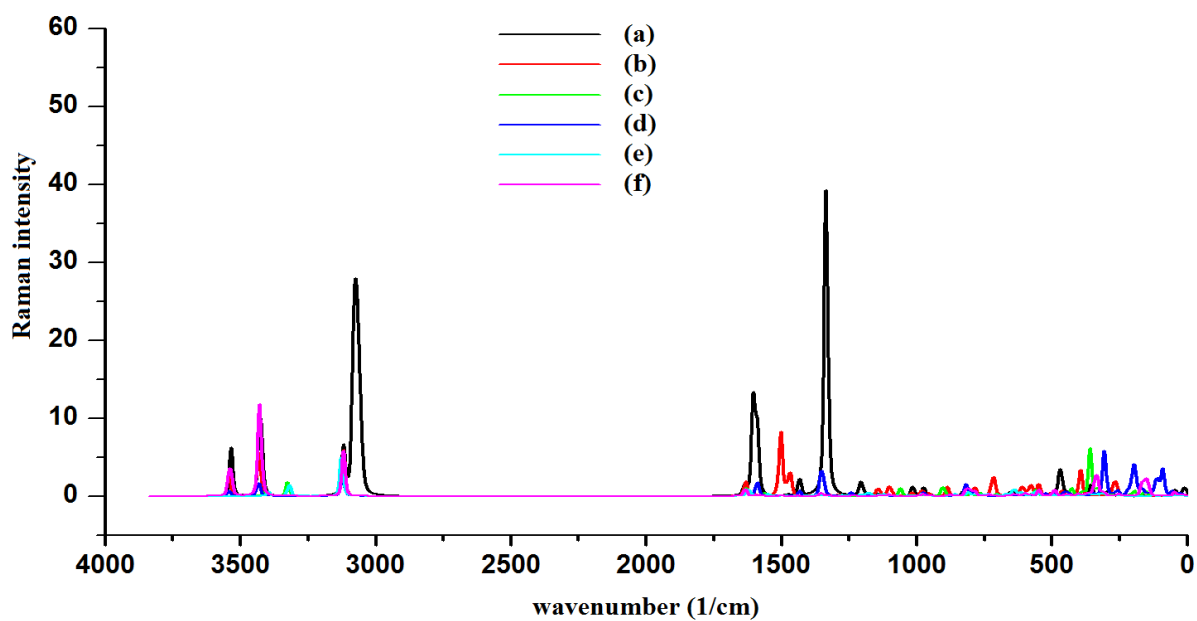


Fig.S4.2 Raman spectrum of (a) G-CA (b) F-CA (c) AlN-CA (d) AlP-CA (e) BN-CA (f) BP-CA

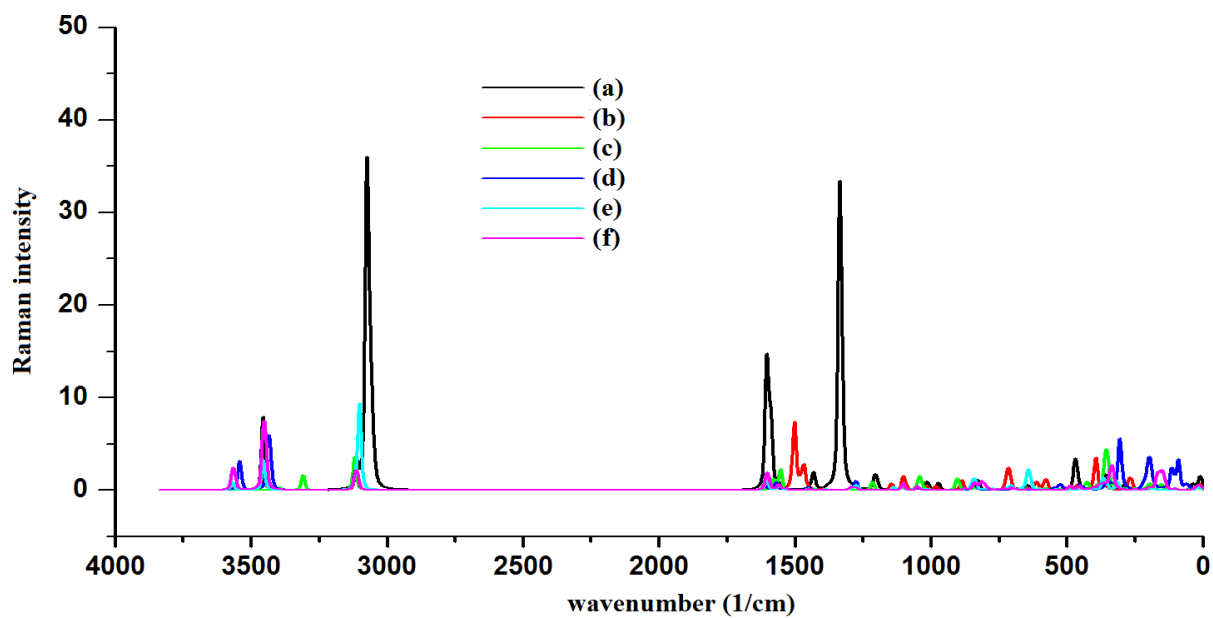


Fig.S4.3 Raman spectrum of (a) G-BA (b) F-BA (c) AlN-BA (d) AlP-BA (e) BN-BA (f) BP-BA

