only 2% of the total oscillator strength. The excitonic coupling shows fluctuations similar to the site energies. Its variance, however, amounts to only 7% of the average value of 0.25eV. Hallermeier et al[4] deduced a smaller excitonic coupling of 0.078 eV. Most probably their dimer spectrum has some admixture of the monomer spectrum. We assume that the absorption maximum at 520nm is due to monomers and the maximum of the real dimer spectrum is at 480nm. This would be consistent with an H-aggregate with an excitonic coupling of 0.2eV.

We studied also brickwork structures as a model for the J-aggregates with a red shifted absorption. We found a relative stable structure which is shown in fig. 3b. The structural fluctuations are much larger than for the sandwich model but the fluctuations of site energies and excitonic coupling are even somewhat smaller. The coupling of -0.064eV is close to the value of -0.078eV which was used to simulate the vibronic spectrum of the J-aggregates[18].

Acknowledgments

This work has been supported by the Deutsche Forschungsgemeinschaft (SFB 533)

---

* Electronic address: philipp.scherer@ph.tum.de

[1] G.Scheibe, Angew. Chemie **49**, 563 (1936)

[2] E.E.Jelley, Nature **138** ,1009 (1936)

[3] B.Neumann, J.Phys.Chem. B **105**, 8268 (2001)

[4] B.Kopainsky, J.K.Hallermeier and W.Kaiser, Chem.Phys.Lett. **83**, 498 (1981)

[5] G.R.Bird,K.S.Norland,A.E.Rosenoff,H.B.Michaud, Phot.Sci.Eng. 12 ,196 (1968)

[6] R.E.Graves, P.I.Rose, J.Phys.Chem. **79**, 746 (1975)

[7] H.J.Nolte, Chem.Phys.Lett. **31**, 134 (1975)

[8] G.Scheibe, Z.Elektrochemie, **52**, 283 (1948)

[9] P.O.J.Scherer, J.Phys.Chem. A **104**, 6301 (2000)

[10] M.W.Mahoney, W.L.Jorgensen, J.Chem.Phys. **112**, 8910 (2000)

[11] I.P.Omelyan, Phys.Rev.E **58**, 1169 (1998)

[12] H.Li, C.S.Pomelli, J.H.Jensen, Theor. Chem. Acc. **109**,71 (2003)