

Abstract Submitted  
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**Complexation of Flavonoids with Iron: Structure and Optical Signatures** JUN REN, SHENG MENG, Physics Department and School of Engineering and Applied Sciences, Harvard University, CH. E. LEKKA, Department of Materials Science and Engineering, University of Ioannina, Ioannina 45110, Greece, EFTHIMIOS KAXIRAS, Physics Department and School of Engineering and Applied Sciences, Harvard University — Flavonoids exhibit antioxidant behavior believed to be related to their metal ion chelation ability. We investigate the complexation mechanism of several flavonoids, quercetin, luteolin, galangin, kaempferol and chrysin with iron, the most abundant type of metal ions in the body, through first-principles electronic structure calculations based on Density Functional Theory (DFT). We find that the most likely chelation site for Fe is the 3-hydroxyl-4-carbonyl group, followed by 4-carbonyl-5-hydroxyl group and the 3'-4' hydroxyl (if present) for all the flavonoid molecules studied. Three quercetin molecules are required to saturate the bonds of a single Fe ion by forming six orthogonal Fe-O bonds, though the binding energy per molecule is highest for complexes consisting of two quercetin molecules and one Fe atom, in agreement with experiment. Optical absorption spectra calculated with time-dependent DFT serve as signatures to identify various complexes. For the iron-quercetin complexes, we find a redshift of the first absorbance peak upon complexation in good agreement with experiment; this behavior is explained by the narrowing of the optical gap of quercetin due to Fe(d)-O(p) orbital hybridization.

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