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Antioxidative mechanism and anisotropic charge transport properties of mangiferin: A theoretical study

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Abstract. A quantum mechanical approach has been used to investigate the antioxidative mechanism for scavenging •OOH and •OH radicals using mangiferin in solution phase. Mangiferin is also used as a potent applicant for organic semiconductor. The charge-transport properties in mangiferin have been studied based on the first-principle DFT combined with the Marcus-Hush theory. Density functional theory (DFT) calculations at the B3LYP/6-311+G(d,p) level were used to optimize mangiferin and its different forms. The lowest theoretical bond dissociation enthalpy (BDE) value for 7-OH site of mangiferin in water, indicates that 7-OH group is important in the antioxidant activity. The relative values of enthalpies also show that oxidation of mangiferin by •OOH and •OH radical is an exothermic process. The predicted maximum electron mobility value of mangiferin is 0.148 $cm^2\ V^{-1}\ s^{-1}$, which appears at the orientation angle near 49°/311° of conducting channel on the reference planes a-b. Theoretical investigation of natural semiconductors is helpful for designing higher performance electronic materials used in biochemical and industrial field to replace expensive and rare organic materials.

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Key words: anisotropic, organic semiconductor, mangiferin, antioxidant, charge transport.

1 Introduction

Mangiferin is a class of polyphenolic compounds, having two benzene ring (A and B) condensed with a six-membered ring (C) (see Fig. 1). Its presence has been investigated in mango, hypericum elegans, and tripterospermum lanceolatum. Mangiferin have attracted attention of many researchers since 1960' because of its widerange appliactions in

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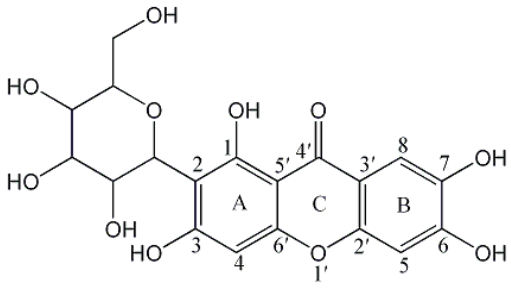

Figure 1: Chemical structure of mangiferin.

biochemical industries [1-9]. Mangiferin bioactivities have been correlated with radical scavenging as well as inhibition of oxidative stress and complex formation with Fe [8,9]. Some natural polyphenolic compounds, such as 3-hydroxyflavone and quercetin, have been used as an additive in solar cell devices [10-12] due to its low cost, easy attainability, and no environmental threat. Mangiferin have become a viable alternative to expensive and rare organic materials. Therefore, in order to elucidate its pharmacological mechanism; use as novel drugs and natural electronic materials investigation of its fundamental chemical behavior and electronic characteristics will be of great significance. Polyphenolic compounds, such as flavonoids, have also been found as potential anti-cancer, anti-inflammatory, antibacterial, antiviral, and antiallergic applicants [13-17]. They prevent biological and chemical substances from oxidative damage by reactive oxygen species and have been used as possible therapeutics against a wide variety of diseases caused by radical damage [15]. Recently, the antimutagenic activity of phenolic compounds, particularly flavonoids such as rutin, have been studied on the basis of their scavenging capability against the free radicals, such as •OH [16]. The reaction can be expressed as $R^{\bullet} + R'OH \rightarrow R'O^{\bullet} + RH$, the formed radical $R'O^{\bullet}$ should be relatively stable so that the reaction becomes thermodynamically favorable [18,19].

Many experimental and theoretical studies about antioxidant properties of polyphenolic compounds have focused on the investigation of flavonoids [18-24]. Recently Lengyel *et al.* [18] and Vaganek *et al.* [19] have carried out calculations for O-H bond dissociation enthalpies, proton dissociation enthalpies, ionization potentials, proton affinities and electron transfer enthalpies related to HAT, SET-PT and SPLET mechanisms in gas and solution-phases of some isoflavones and flavonoids. The electrical anisotropy as an intrinsic property of organic semiconductors has aroused the attention of many researchers [25-30] A strong anisotropy of the field-effect mobility with the a-b plane of single crystals of rubrene has been observed by Sundar *et al.* [28]. Direct and inverse photoemission spectroscopy and some other experimental methods have been performed to study the n-type doping of a variety of electron transport materials by Kahn and coworkers [31-36]. Although there are several computational studies for the electrical anisotropy [37-40], a systemic investigation of anisotropic mobilites is still lacking. Based on Marcus-Hush theory [41,42], Han and coworkers have developed a method to simulate the angular res-