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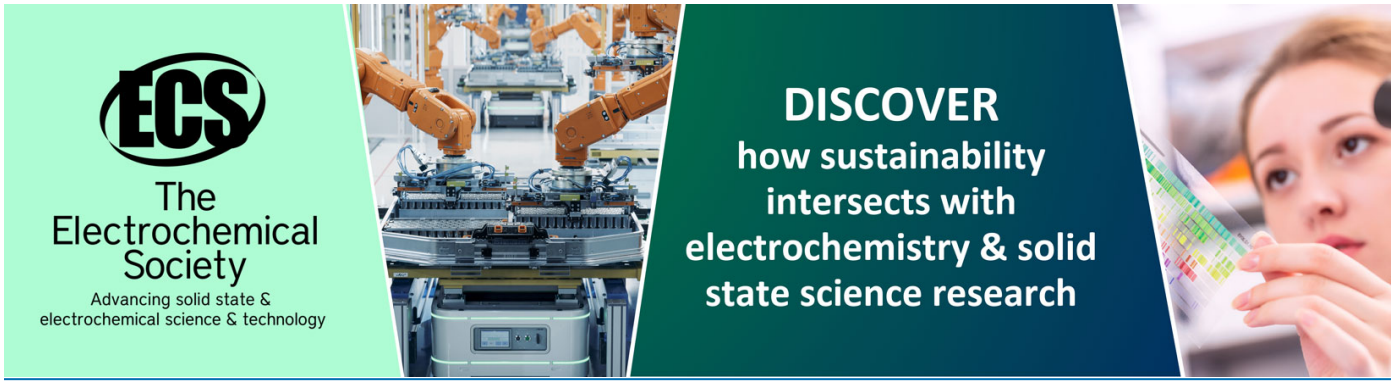

Investigation of electron scattering asymmetries in halocamphors

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Synopsis We present a study on the electron transmission and dissociative electron attachment asymmetries in halocamphor species. Our results consist in their anion state spectra, applied in a model for the spin-polarized electron scattering problem under the influence of a low energy resonance.

Motivated by the Vester-Ulbrich hypothesis for biological homochirality [1], chiral sensitivity in longitudinally-polarized spin electron scattering has been investigated in the last decades. Electron transmission asymmetry experiments reported by Mayer *et al.* show that the magnitude of scattering asymmetries for Bromocamphors are enhanced by the formation of resonances, in a phenomenon called electron circular dichroism (ECD) [2].

More recently, the dissociative electron attachment (DEA) asymmetries for 3-Bromocamphor (3BrC), 3-Iodocamphor (3IC) and 10-Iodocamphor (10IC) were reported by Dreiling *et al.* [3]. The results obtained do not seem consistent with theoretical predictions, and points out the need for the development of a new model to provide an understanding of the magnitudes and energy dependence of the asymmetries.

We investigated the temporary electron attachment in the halocamphor molecules by elastic scattering calculations using the Schwinger multichannel method with pseudopotentials (SMCPP) [4]. The anionic spectra were analyzed and their resonances were characterized, from which provided essential information to understanding the expected dissociation mechanisms and the related chiral asymmetries.

A model, proposed elsewhere, is being developed for the spin-dependent electron scattering problem under the influence of a low energy resonance. Provided that the anion state spectra are known, we intend to explain the experimental results of asymmetries.

The electron transmission asymmetry for 3-Bromocamphor was computed in a first, preliminary calculation, which considered its anion spectra (Table 1). Figure 1 shows the obtained results and indicates a qualitative agreement with the experimental data measured by Mayer *et al.*[2].

Table 1. Energies of anionic states and widths (in parenthesis), in eV, obtained from SMCPP calculations. States are labeled according to orbital character.

	σ_1^*	σ_2^*
3-Bromocamphor	0.32 (0.192)	2.34 (0.49)
	σ^*	π^*
3-Iodocamphor	-0.01	2.00 (0.50)
10-Iodocamphor	0.25 (0.03)	1.77 (0.19)

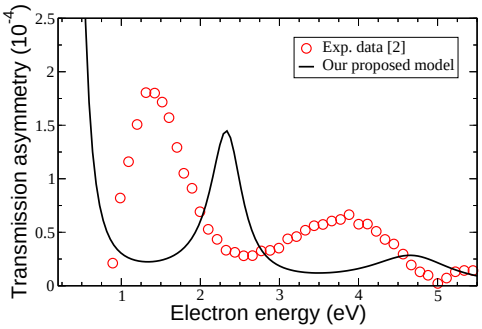

Figure 1. Asymmetry obtained by our model against experimental data [2], for 3BrC.

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References

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