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Developing a Methodology for Systematic Selection of Probe Liquids to Determine Hansen Solubility Parameters for Carbon Black materials

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Hansen Solubility Parameters (HSP) are particularly relevant when focusing on the dispersion of particles and offer valuable insights into the surface characteristics of nanoparticles [1,2]. HSPs can provide understanding into integral factors in the meticulous design of electrodes, electrolytes, and other pivotal components inherent to electrochemical systems. However, current methods for determining HSP through the sedimentation of nanoparticles involve the use of multiple probe liquids, leading to time-consuming, expensive experiments with potential health risks. In response to this challenge, we developed a two-step strategy that facilitates a systematic selection of liquids (Figure 1).

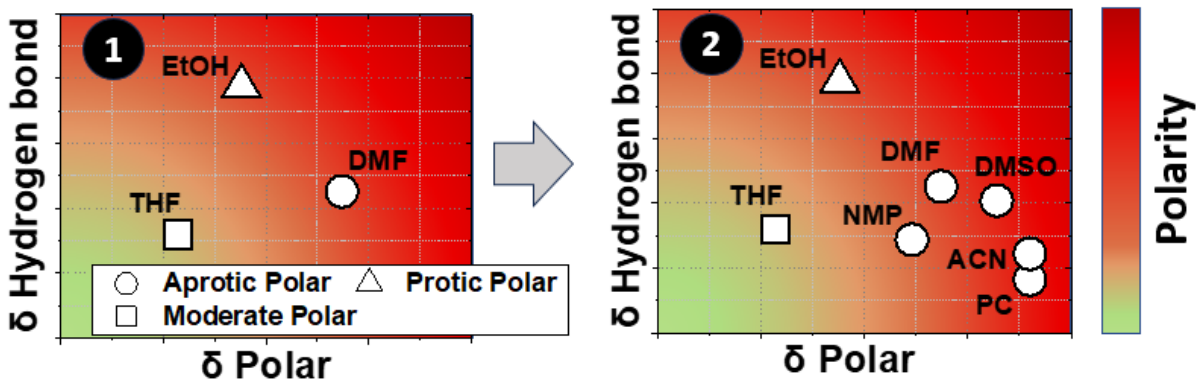

Figure 1: Procedure for the rational selection of probe liquids for determining HSP.

The pivotal aspect of this approach involves initially identifying the approximate location of the Hansen sphere in the three-dimensional interaction space using a carefully selected set of probe liquids with varying polarities and chemical structures. Subsequently, based on the outcomes of the first step, a specific set of liquids is chosen for the final determination of HSP (Figure 1).

Collectively, the implemented procedure diminishes the necessary liquid volume for experiments, cutting it down from the current requirement of over ten to a maximum of seven. This selection is determined through a well-defined, cohesive methodology. The validation process encompassed various materials such as carbon black, non-pigmentary nano-scale titania, silicon/carbon composites, and lanthanum cobaltite particles. These materials are widely employed in applications like fuel cells, batteries, cyclohexene oxidation, catalytic combustion, photocatalysis, and heterogeneous Fenton reactions.

For the case of carbon Black, the interaction between 13 probe liquids and four analysed carbon black types, namely Super C65 (C65), Ketjenblack 300 (KB300), Ketjenblack 600 (KB600) and Vulcan XC72R (XC72R) was investigated. Across all four materials, it is observable that carbon black interacts effectively, except for non-polar probe liquids. The majority of probe liquids identified as beneficial for interacting with carbon black belong to the categories of moderate polar liquids (Ethyl Acetate, Tetrahydrofuran, Acetone) and aprotic polar liquids (Dimethyl Formamide, N-Methyl-2-Pyrrolidone, Dimethyl Sulfoxide).

Based on the findings, the amount of probe liquids to end up in a HSP could be significantly reduced by applying the developed two-step strategy. Despite the reduction in the probe liquids list, the HSP values have not changed significantly.

The study highlights three distinct advantages. Firstly, the liquid selection approach expedites the process by focusing on experiments with probe liquids that demonstrate optimal interaction with the substance of interest. Notably, these interactions play a crucial role in the ultimate derivation of HSP. Secondly, the structured methodology enhances comparability among HSP determined by various researchers. This is achieved by establishing a defined systematic for probe liquid selection, alleviating the operator from subjective decisions on which probe liquids to employ or avoid. Lastly, categorizing probe liquids based on their polarity facilitates an intuitive and physical comprehension of the pertinent interfaces at play.

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