Technical Manuscript Writing for Doctoral Candidates

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Module 13. The Abstract

The abstract is critically important part of the paper. Remember that all that many people will read of your paper is the abstract. If it looks good and interesting, then they may read more.

I. Parts of the Abstract

The abstract performs three functions.

- provide the background of the problem (one or two sentences)
- summarize the methodology (one sentence)
- summarize the important results (one or two sentences)
- highlight the significance of the work (one sentence)

II. Contents of the Results and Discussion Section

We now examine several abstracts.

There are three examples given on the final page of the Journal of Physical Chemistry Author Guide, which is provided on the course website. We also examine the abstracts of the two example manuscripts.

Example 1. A Theoretical Manuscript
[Wang *et al.*, *Phys. Rev. E* **81** 061204 (2010)]

background

In this work, we test the ability of the Ornstein-Zernike equation in the Percus-Yevick approximation (OZPY) to generate interaction potentials from pair correlation functions (PCFs) of monatomic and diatomic Lennard-Jones fluids.

method

The PCFs are generated by solving OZPY equation (monatomic fluid) and molecular dynamics (MD) simulations (diatomic fluid). Since the interaction potentials are inputs in the OZPY method and the MD simulation, the extraction of the potential from the PCFs using OZPY is a test of self-consistency. This test is necessary if the procedure is to be used to generate coarse-grained (CG) potentials from PCFs.

results

We find that the procedure is completely self-consistent for the monatomic fluid in the whole range of densities studied (reduced density up to 0.55, under reduced temperature of 2.0). In the diatomic case, we find that the procedure is generally self-consistent under both low and high densities, although there is a systematic deviation at high densities. The method is able to reproduce the two parameters σ and ε of the input Lennard-Jones potential model to within about 1%.

significance

This CG potential generating procedure can be straightforwardly extended to more complicated molecules.

Example 2. An Experimental Manuscript
[Liu *et al.*, *Chem. Eng. J.* **151** pp. 235-240 (2009)]

background

We prepared Fe3O4 particles and two types of composite magnetic particles derived from Fe3O4 and bis(trimethoxysilylpropyl)amine (TSPA), and from Fe3O4 and a flocculating agent 1010f (a copolymer of acrylamide, sodium acrylate, and [2-(acryloyloxy)ethyl]trimethylammonium chloride). Using these particles, boron adsorption in aqueous solution was comprehensively investigated.

results

The adsorption was found to occur rapidly in the first 2 h and the particle composition did not have a significant effect on the equilibrium time. We found that Fe3O4–TSPA particles presented the highest adsorption capacity, whereas the pure Fe3O4 particles showed the lowest capacity. For all particles, amount of boron adsorption decreased with the initial pH in the order of 6.0 > 2.2 > 11.7. In general, the adsorption amount appeared to decrease with the increase in ionic strength.We propose that boron is adsorbed in the form of bothH3BO3 and B(OH)4 −through the interactions of hydrogen bonding, electrostatic and hydrophobic attractions.

significance

The information gained in this study would be helpful for both understanding the adsorption mechanism and designing low-cost and easily available adsorbents for boron.