

Supervisor's statement upon Ph.D. thesis

“The study of the association behaviour of the amphiphilic copolymers in solutions containing low molar compounds by means of computer simulation” by Mgr. Karel Šindelka

Studium asociačního chování amfifilních kopolymerů v roztocích obsahujících nízkomolekulární látky pomocí počítačových simulací

I know Karel Šindelka since his bachelor studies at the Department of Physical and Macromolecular Chemistry of Faculty of Science, Charles University, Prague. In 2014 he defended his Master thesis “Self-assembly of polyelectrolytes in aqueous solutions (dissipative particle dynamics, DPD)” elaborated under my supervision.

After graduation, he started PhD. study at our group under my supervision. The study of complex polyelectrolyte solutions required appropriate relationship of individual effects, i.e. of the soft repulsive potentials (describing the amphiphilic interactions) and electrostatic potentials. He solved this peculiar task and properly mapped DPD data on the experimental results of the pH-dependent self-assembly of a diblock copolymer, poly(2-vinylpyridine)-block-poly(ethylene oxide) in aqueous solutions. and so simultaneously showed that the DPD method is a suitable simulation technique for studying the global properties of complex polyelectrolyte solutions. These results were published in *Macromolecules* in 2016 and as this study proved that the DPD method is a suitable simulation technique for studying the global properties of complex polyelectrolyte solutions this paper was cited 37 times according to WoS.

Karel Šindelka applied DPD method with this parameterization to simulations of several other polyelectrolyte systems (three original papers published in impacted international journals) and his results were summarized in two review articles, e.g. invited review in *Molecular Physics*. He published 6 papers in impacted international journals, his H-index according WoS is 4 and he also presented several oral talks and posters on international conferences. According to WoS, the average citations per item is 11,71 and sum of times cited without self citations 67. As the greater part of the papers citing K. Šindelka's research are experimental ones, I am sure that the obtained results are very useful not only from the methodological point of view but also for the interpretation of experimental studies in general.

During his PhD study, he spent three months in the group of Prof. T.M. Birshtein at Saint Petersburg University, Russia. As the principal investigator of the grant number 422216, ‘Study of complexation between nanoparticles and polyelectrolytes’, of the Grant Agency of the Charles University he applied DPD method to the aqueous solutions of amphiphilic copolymers and inorganic nanoparticles coated by oligomers and studied the stabilization of the formed nanoparticles. He showed that a small excess of copolymer chains is sufficient to prevent macroscopic phase separation, stabilizing the aqueous dispersions. This finding is important from the application point of view as stable aqueous dispersions are necessary for successful application of hybrid organic-inorganic nanoparticles.

According to my opinion, the PhD thesis is written at a good scientific and language level. The dissertation thesis clearly demonstrates the high qualification of the candidate and his ability to carry out scientific research independently.

The thesis complies with all requirements on PhD thesis and I strongly recommend the thesis for the defense. Mgr. Karel Šindelka is certainly one of my best students. Karel Šindelka is really talented and devoted young scientist with a deep background in computer simulations of polyelectrolytes.

In Prague, August 3, 2018

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