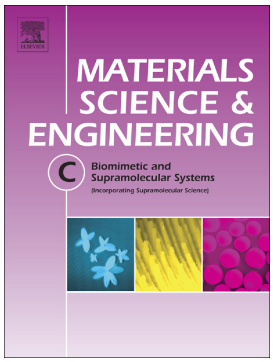

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Synergetically understanding the interaction between nano/microspheres and peptide for controllable drug loading via experimental and theoretical approaches

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Abstract: In this paper we systematically investigate the loading capacity of raspberry–like nano/microspheres with highly cross–linked structure for the peptide, immunostimulating hexapeptide from human (IHH), by integrating both experimental and simulation efforts. The experimental results indicate that the loading capacities of raspberry–like nano/microspheres with different functionalized chains vary drastically. To provide theoretical insights into the observed phenomenon, the typical raspberry–like nano/microspheres were simplified as effective functionalized groups, thereby the interactions between them and IHH were accurately calculated by *ab initio* method. The *ab* initio results agree well with the experimental observations, and the underlying binding mechanism are analysed in great details. It is shown that hydrogen bonding plays an important role and the binding affinity strongly depends on the functionalized motifs. Therefore, this work provides insightful guidance to controlling the drug loading by design of the functionalized surface of nanomaterials.

Keywords: *nano/microspheres, highly cross–linked, drug peptide, binding, ab initio*