Universal criteria for designability of heteropolymers

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Heteropolymers are important examples in material science of self-assembling systems. The technology for the synthesis and manipulation of such heteropolymers is already advanced, and it is nowadays possible to synthesize polymers made of up 7 different monomers with complex pattern arrangements (e.g. block copolymers) [1,2]. However, it is still not possible to design heteropolymers with control over the single chain self-assembling properties comparable to what natural bio-polymers, such as DNA and proteins, can achieve. Here we introduce a criterion to discriminate between polymers that can be designed to adopt a predetermined structure from polymers that cannot, and show that this criterion is fulfilled by the addition of few directional interactions to the monomers of the chain. The criterion is based on the appearance of a particular peak in the radial distribution function that dominates over the random packing of the heteropolymer. We show that the presence of such a peak indicates that it exists at least one pattern that will drive the system to collapse towards a specific target structure. Moreover, we show that the peak is a universal feature of all designable heteropolymers, as it is dominating also the radial distribution function of natural proteins. The criterion that we present can be applied to engineer new types of self-assembling modular polymers that will open new applications for polymer-based materials science.
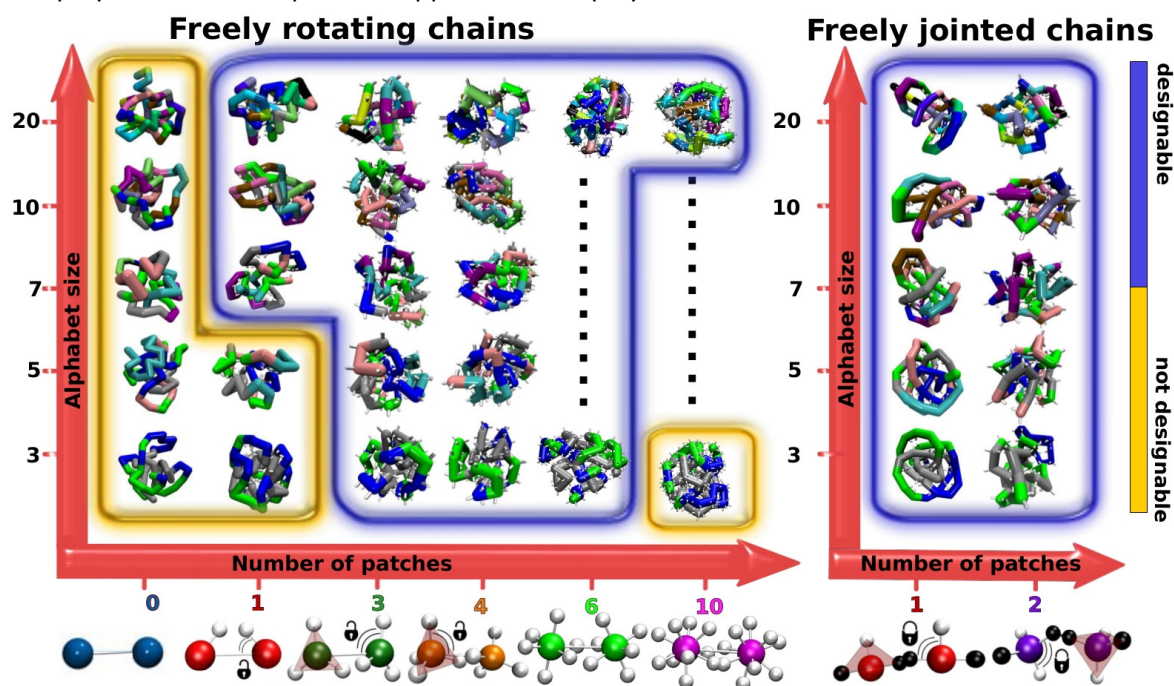
Figure1 Designability diagram for each patch number for freely rotating chains (left) and freely jointed chains (right), for different alphabet sizes. For each case, the chosen target structure is shown. The systems in the blue area are designable, the ones in the yellow area are not designable and the one in the green area is borderline. When the number of patches increases the interactions are again isotropic, such as in the case without patches.

[1] T. P. Lodge, *Macromolecular Chemistry and Physics* , 2003, **204**, 265.
[2] A. Hirao, T. Higashihara, and K. Inoue, *Macromolecules* , 2008, **41**, 3579.