Supplementary Information for Optimising Minimal Building Blocks for Addressable Self-Assembly

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I. EXAMPLE DESIGNS

Here, we provide illustrations of some more examples of optimised interfaces. Figure S1 shows three possible designs for a system that requires three binding interfaces. Four possible approaches are shown: two use only one type of patch (first and third columns), while two use distinct patches with exclusive interactions, indicated by different colours (second and fourth columns). The first two columns use three patches per face, while the last two use five.

Figure S2 shows the analogous interface designs for a larger set of 13 interfaces, which is the number required for the Vitruvian man structure in the main article. In practice, identical patches do not lead to viable self-assembly. The performance of the designs with distinct patch types (and other arrangements with three and five patches) is discussed in Section 4.2.3 of the main article.

Optimised patch coordinates for all combinations of 3–20 interfaces and 3–5 patch types are available as supporting data at doi:10.15128/r26682x3950

II. RESTRICTED PATCH ALPHABETS

In the main article, interfaces were designed and tested with two sorts of interaction "alphabets". In the first case, the alphabet was minimal and all patches were equivalent. In the second case, all patches on a given face were of distinct types, and patches of different types did not interact. This choice gives an alphabet size equal to twice the number of patches per face, once the complementary patches on the binding partners are taken into account.

Here, we briefly consider the intermediate case where distinct patches are present, but the number of types is less than the number of patches per face. Some types of patches therefore appear more than once on each face. Figure S3 shows yields of addressable dimers, calculated in the same way as in the main article, but with the alphabet restricted to three distinct types plus their complements on binding partners. For designs with $n_{\mathrm{p}} = 3$ patches for face (red line), all patches on a given face are distinct and the results are identical to Fig. 6 of the main article. This provides a reference for the minimum number of patches with this size of alphabet. The solid blue and green lines for the cases of 4 and 5 patches per face with matching alphabet sizes are also reproduced from Fig. 6. The dashed blue and green lines show the cases of 4 patches per face (with one patch type repeated) and 5 patches per face (with two patch types repeated). We see that deploying additional patches without increasing the alphabet size does provide

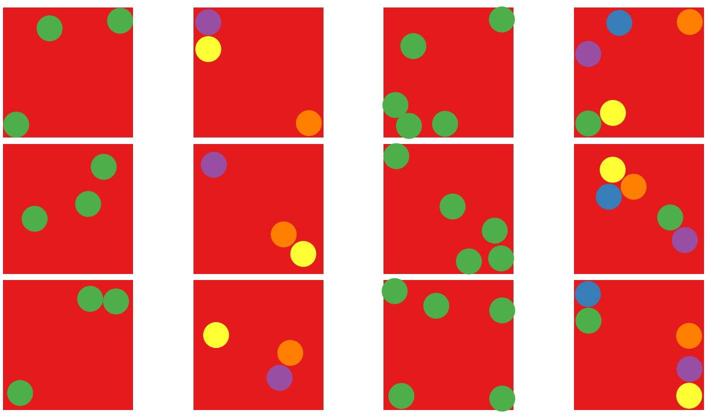

FIG. S1: Example optimised designs for three interfaces. Columns from left to right: designs using three identical patches, three distinct patch types, five identical patches, and five distinct patch types. Each interface has a binding partner with a mirror-image pattern of patches.

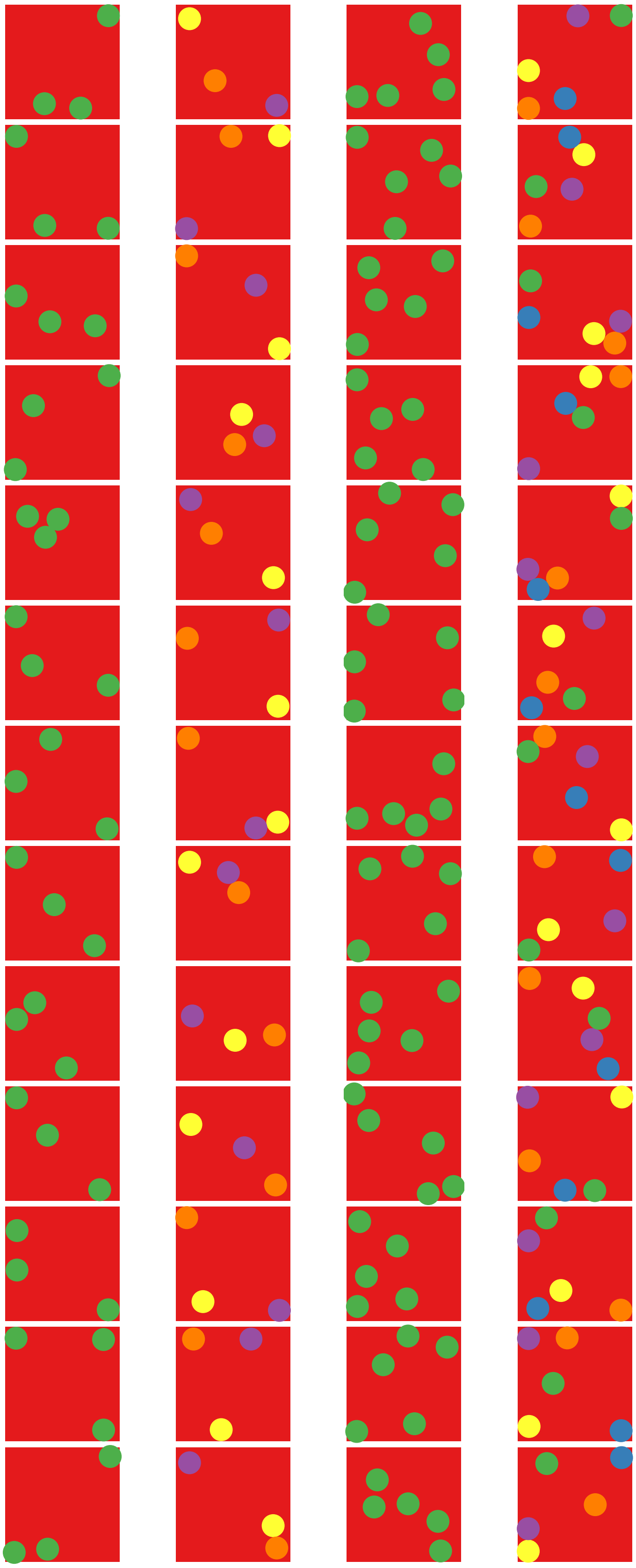

FIG. S2: Example optimal designs for thirteen interfaces, which is the number required to construct the Vitruvian man target. Designs are shown for three and five patches per face, using identical (green) and distinct (multi-coloured) patch types. Each interface has a binding partner with a mirror-image pattern of patches.

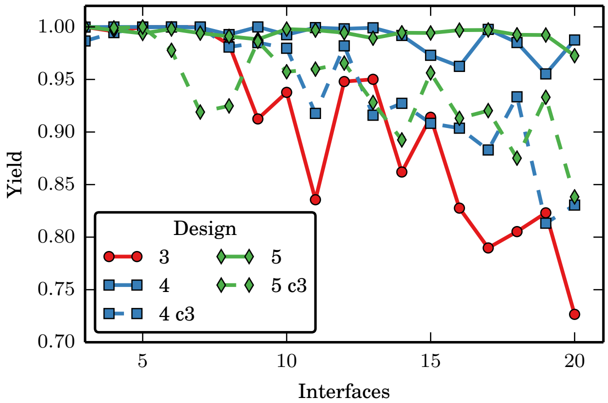

FIG. S3: Yields for sets of dimers where dashed lines indicate designs restricted to three unique colours on a given face.

some improvement in performance, but designs where the alphabet size matches the number of patches per face are considerably better.

On the basis of this observation, we may also predict that it would not be advantageous to lift the restriction of one patch of each type per face in cases where the number of patches per face matches the alphabet size (such as the second and fourth columns in Figs. S1 and S2). Although such a change appears to provide greater flexibility in the design process, the introduction of identical patches on the same face immediately stabilises unwanted configurations where building blocks are bound in incorrect orientations by pairs of patches. This is the effect that limits the improvement gained by increasing the number of patches without increasing the alphabet size in Fig. S3.