## Reinforcement Learning-based Design of Shape-changing Metamaterials

Sergi Bernaus Oliva<sup>1†</sup>, Felix T. Bölle<sup>1†</sup>, A.T.Las<sup>1</sup>, Xiaoxing Xia<sup>2</sup> and Ivano E. Castelli<sup>1</sup>

<sup>1</sup>Department of Energy Conversion and Storage, Technical University of Denmark, Street, Anker Engelundsvej 411, DK-2800, Kgs. Lyngby, Denmark. <sup>2</sup>Materials Engineering Division, Lawrence Livermore National Laboratory, 7000 East Ave., Livermore, 94550, California, USA.

<sup>†</sup>These authors contributed equally to this work.

## Supplementaty Information



Fig. S1 Render displaying how the rotation can take place in a 3d structure, where the pillars are rotated rotating all the layered 2d beams together.

Figure S1 shows how the beams change from a non-lithiated state (a) to a lithiated (bent) state (b) with arrows indicating the direction of rotation for each of the beams. This simulation render represents 3 layers of the 30 degree canvas generated by the algorithm stacked on top of each other.



Fig. S2 Results of training using 30 degrees adjusted with (a) and without (b) frustration with the higher final score than the closed canvas counterpart.

Figure S2 shows the results of the training using 30-degree increments adjusted. Instead of the adjustment providing a closed shape as designed, the algorithm finds an alternative shape which maximises the score without producing a closed shape. The score is significantly higher than the closed alternative using the same input parameters (4.62 vs 4.24), but in exchange, the final structure is more complex and has lower expected stability and cyclability.



Fig. S3 Images of the experimentally tested PDMS lattices before and after swelling.

Figure S3 shows images of the experimentally tested PDMS lattices before and after swelling by a solvent. We first tested a square lattice that is similar to the ones in [1], and it transformed to a sinusoidal pattern after swelling as expected. For the square lattice, the node spacing is 20mm; for the MLpredicted non-frustrated lattice, the node spacing is 20mm in the x direction and 10mm in the y direction; for ML-predicted frustrated lattice, the node spacing is 26mm in the x direction and 13mm in the y direction. For all designs, the beam width is 2mm and the beam thickness in the z direction is 4mm, and the nodes are approximated by doughnut-shaped rings with an inner diameter of 2mm and an outer diameter of 6mm. Before the swelling experiments, the PDMS lattices are mounted onto a 3D-printed base plate with vertical posts that are inserted into all doughnut-shaped nodes. In doing so, the lateral positions of all the nodes in the PDMS lattices are constrained but the nodes are free to rotate in the right-handed or left-handed directions.

## References

 Xia, X., Afshar, A., Yang, H., Portela, C.M., Kochmann, D.M., Di Leo, C.V., Greer, J.R.: Electrochemically reconfigurable architected materials. Nature 573(7773), 205–213 (2019)