Light Causes This Fibre to Bend!

MD Model of Photosensitive Molecular Motors

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Conclusion

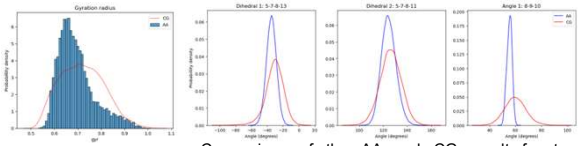
We have constructed an all-atom (AA) and a coarse-grained (CG) model for fibres and fibre bundles made from photosensitive molecular motors and characterised the microscopic behaviour of the system. We show that the fibre volume remains the same, and that motors pack closer together after photoactuation – both possible explanations for macroscopic bending.

Report & Animations

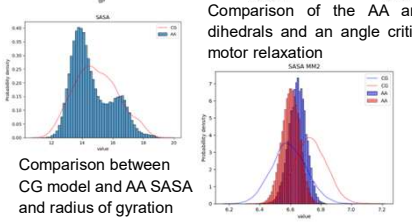
Background

In 2017, the Feringa group described an “Artificial muscle-like function from hierarchical supramolecular assembly of photoresponsive molecular motors”, a fibre that bends when illuminated. The supramolecular assembly consists of many aligned fibres connected by ionic interactions. They observed that the fibre radius increased after actuation and hypothesised that the volume remain constant so that the radius increase leads to fibre contraction. Since only the fibres on the side of the bundle facing the light source contract, the bundle bends towards the light.

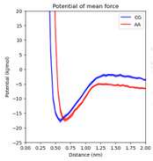
Model Validation



Comparison of the AA and CG result for two dihedrals and an angle critical for the rotation and motor relaxation



Comparison between CG model and AA SASA and radius of gyration



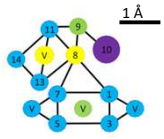
The CG model does not capture packing differences between A and B

SASA comparison. A (*blue*), B (*red*) motor for AA (*bars*) and CG model (*line*). Differences between A and the B are too small to be captured by the CG model.

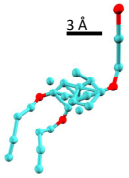
System Description and Characterisation

- Motors inside the fibre are strained and display very different behaviour compared to motors in solution.
- The ground-state motor (A) and the actuated motor (B) have the same volume per motor.
- Motors in the bundle move between fibres at a correlation time of 100 μs/motor.
- Actuated motors (B) pack 10% closer than ground-state motors (A).

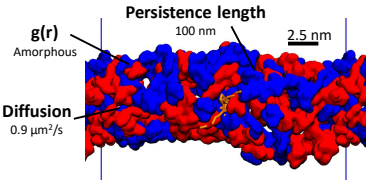
CG



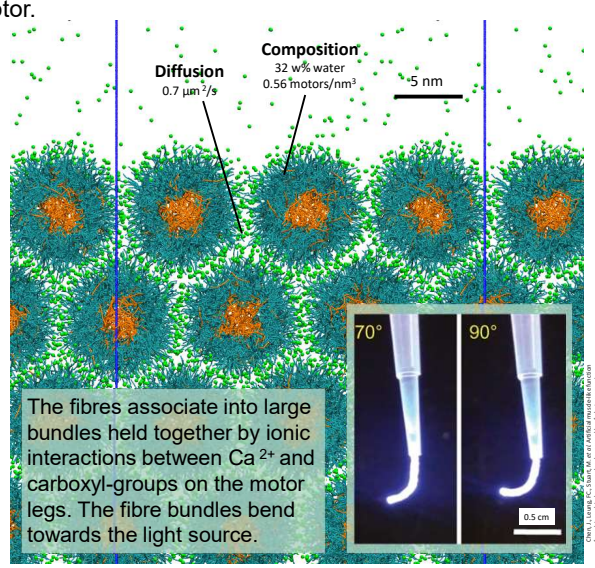
Molecular motor core Rotates 180° around 1’-9 double bond on actuation.



With two polar legs (*blue*) and a non-polar head (*red*), the functionalised motor is amphiphilic.

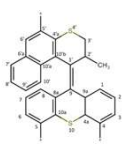


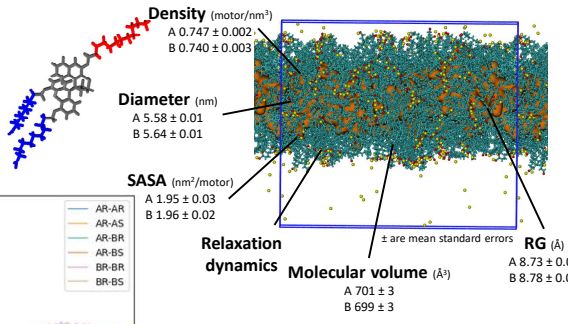
The motors form μm long fibres in water. Experiments show that the radius is 5.4-5.6 nm. The fibres consist of two stereo-isomers (*red* and *blue in* the *upper image*).

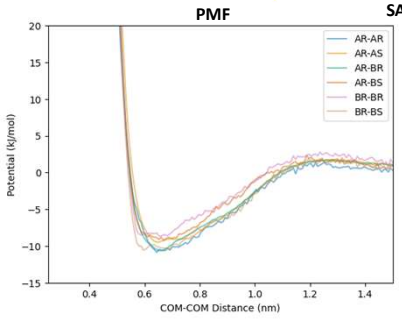


The fibres associate into large bundles held together by ionic interactions between Ca^{2+} and carboxyl-groups on the motor legs. The fibre bundles bend towards the light source.

AA







Potential of mean force governing the distance between two motor cores. **A:** Ground-state motor, **B:** Actuated motor, **R/S:** Stereoisomer for a given molecule. The actuated motor packs closer to its stereoisomer (BR-BS) than any possible packing involving a ground-state motor

Acknowledgements

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