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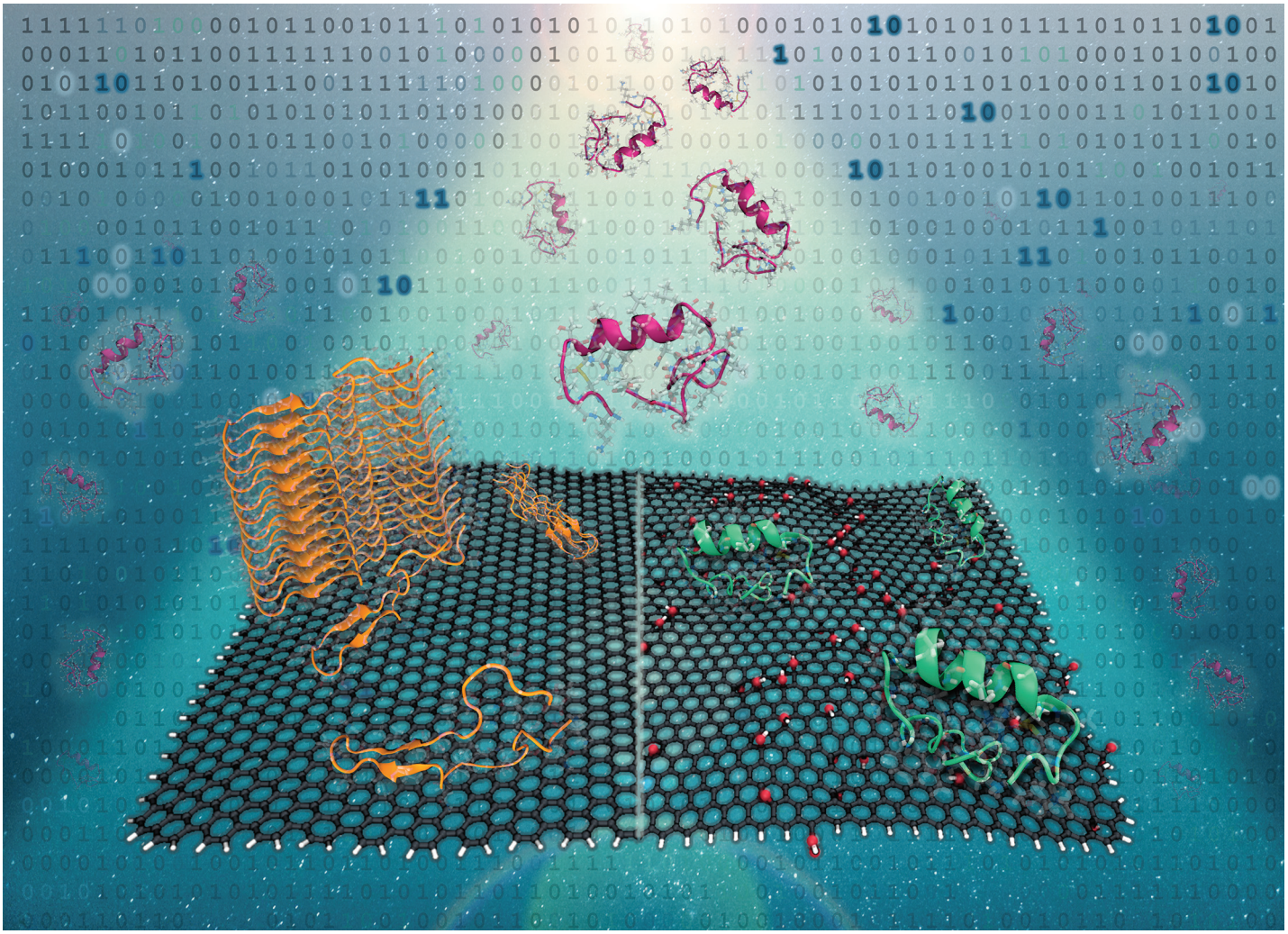


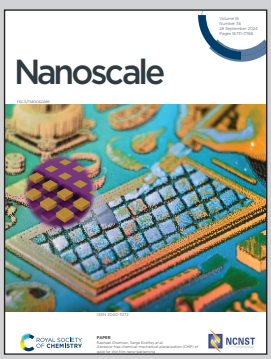
Showcasing research from the Materials Modelling and Simulations Group, RMIT University, Melbourne, Australia.

Graphitic nanoflakes modulate the structure and binding of human amylin

Enhanced sampling molecular dynamics simulations were conducted to explore the structure and adsorption behavior of amylin on graphitic nanoflakes, varying in size and surface functionalization. The study reveals that specific modifications in the nanoflake's dimensions and surface characteristics promote selective and stable protein binding, which in turn influences fibril formation.

These atomistic insights offer important considerations for the design of graphitic nanoflakes capable of modulating protein aggregation, and as such present new avenues for the prevention or management of amyloid-related diseases.

As featured in:



See Nevena Todorova *et al.*, *Nanoscale*, 2024, **16**, 16870.

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