

IN THIS ISSUE

ISSN 2058-9689 CODEN MSDEBG 10(7) 497–600 (2025)



Cover

See Arkalekha Mandal,
Chris Erik Mohn et al.,
pp. 519–533.
Image reproduced by
permission of Arkalekha Mandal
from *Mol. Syst. Des. Eng.*, 2025,
10, 519.



Inside cover

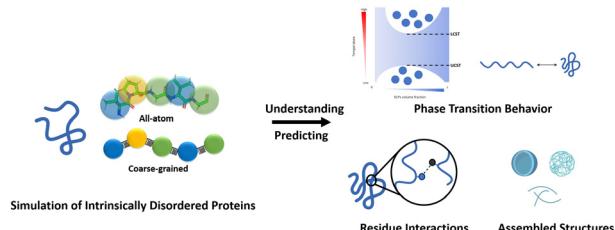
See Bret D. Ulery et al.,
pp. 534–548.
Image reproduced by
permission of The Curators of
the University of Missouri from
Mol. Syst. Des. Eng., 2025,
10, 534.

REVIEW

502

Toward understanding biomolecular materials comprising intrinsically disordered proteins via simulation and experiment

Bin Wang, Tianren Zhang, Sirui Shen, Darrin J. Pochan,
Jeffery G. Saven* and Kristi L. Kiick*

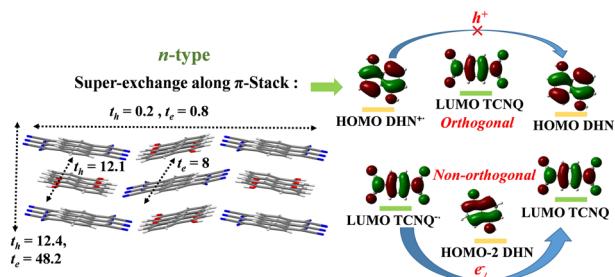


PAPERS

519

Elucidating the role of charge transfer on semiconductor properties in a new donor–acceptor cocrystal 1,5-dihydroxynaphthalene : TCNQ

Arkalekha Mandal,* Chris Erik Mohn,*
Carl Henrik Görbitz, Melania Rogowska and Ola Nilsen





ROYAL SOCIETY
OF CHEMISTRY

GOLD
OPEN
ACCESS

RSC Applied Polymers

The application of polymers, both natural and synthetic

Interdisciplinary and open access

rsc.li/RSCApplPolym

Fundamental questions
Elemental answers

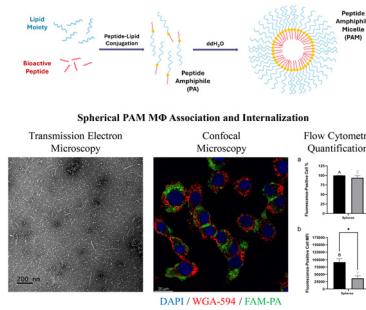
Registered charity number: 207890

PAPERS

534

Vasoactive intestinal peptide amphiphile micelle material properties influence their cell association and internalization

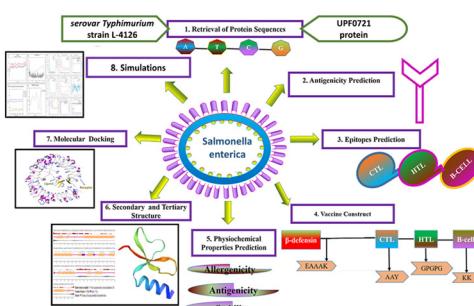
Xiaofei Wang, Agustin T. Barcellona, Fateme Nowruzi, Kambrie M. Brandt, Megan C. Schulte, Luke E. Kruse, Eric Dong, Adam G. Schrum, Esma S. Yolcu and Bret D. Ulery*



549

Designing a multi-epitope vaccine targeting UPF0721 of meningitis-causing *Salmonella enterica* serovar Typhimurium strain L-4126 by utilizing immuno-informatics and *in silico* approaches

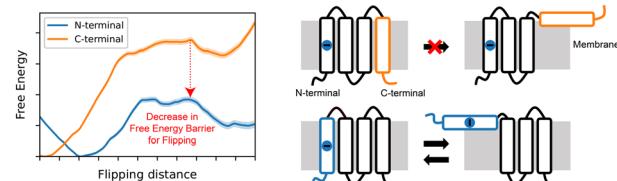
Elham Mohammed Khatrawi, Syed Luqman Ali,* Syed Yasir Ali, Aigul Abduldaiyeva* and Alaa S. Alhegaili



567

Bioinspired design rules for flipping across the lipid bilayer from systematic simulations of membrane protein segments

ByungUk Park and Reid C. Van Lehn*



585

DynaMate: leveraging AI-agents for customized research workflows

Orlando A. Mendible-Barreto, Misael Díaz-Maldonado, Fernando J. Carmona Esteva, J. Emmanuel Torres, Ubaldo M. Córdova-Figueroa and Yamil J. Colón*

```

1 class HelloWorld_inps(BaseModel):
2     message: str = Field(description="Message to print")
3     times: int = Field(description="Amount of times to print message")
4
5
6     def hello_world(message: str, times: int):
7         return message * times
8
9
10    HelloWorld_Tool = StructuredTool.from_function(
11        func=hello_world,
12        name="HelloWorld",
13        description="Prints a message a number of times",
14        args_schema=HelloWorld_inps,
15        return_direction=False,
16        handle_error=True,) 
```

