Protein folding/unfolding phenomenon is originated by synchronization/desynchronization of oscillatory phases of the van der Waals dispersion interaction. A hypothesis.

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Protein Folding Cooperativity.

- Cooperativity in protein folding is generated by an immense set of small interactions, operating in consort, so if one or a small group of those interactions is perturbed the whole network is affected.

- Nowadays the precise object underpinning this cooperativity remains unidentified.

- In this work: **A general mechanism is hypothesized proposed in which two opposed operative actions -synchronization/desynchronization- acts to modulate the state -folded/unfolded- of the same object, a protein.**

- This mechanism operate by changes in van der Waals interaction regime.

Suggestive evidence :

Perspectives in Biochemistry

Dominant Forces in Protein Folding

Ken A. Dill
Department of Pharmaceutical Chemistry, University of California, San Francisco, California 94143-1204
Received April 3, 1990; Revised Manuscript Received May 2, 1990

THE PROTEIN SOCIETY

Clusters of isoleucine, leucine, and valine side chains define cores of stability in high-energy states of globular proteins: Sequence determinants of structure and stability

Sagar V. Kathuria, Yvonne H. Chan, R. Paul Nobrega, Ayşegül Özen, and C. Robert Matthews*

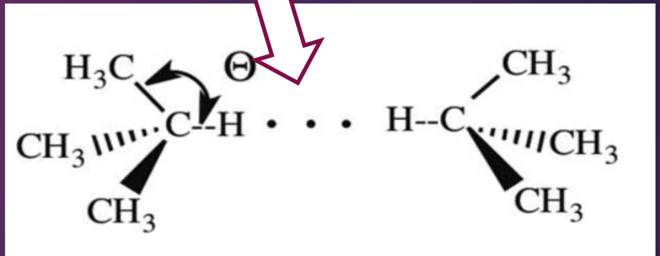
- In proteins the main stabilization cames from hydrophobic aromatic *alkylic* interactivos ILE, VAL & LEU

At the same time → Dihydrogen Bond *in alkyls* act as "Sticky Fingers"

JCTC Journal of Chemical Theory and Computation
Article
pubs.acs.org/JCTC

Understanding the Nature of the CH···HC Interactions in Alkanes

David Danovich,† Sason Shaik,*,† Frank Neese,‡ Jorge Echeverría,§ Gabriel Aullón,§ and Santiago Alvarez*,§



By an alternanting charge $C^{+}H^{-}\cdots H^{+}C^{-}$ / $C^{-}H^{+}\cdots H^{-}C^{+}$ mechanims that gives rise to the London dispersion interactions (Danovich 2013)

Also…

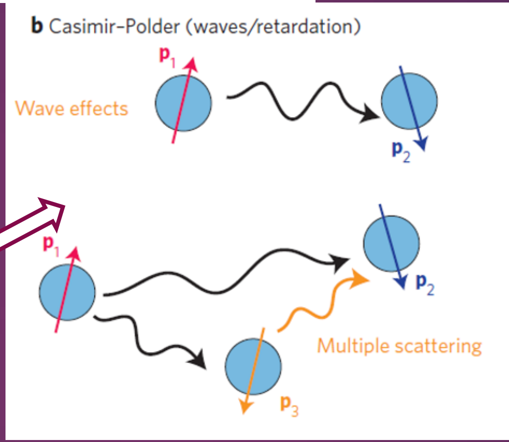
More evidence ....

Van der Waals dispersion is not constant !

The Casimir effect in microstructured geometries

Alejandro W. Rodriguez[1,2], Federico Capasso[1*] and Steven G. Johnson[2]

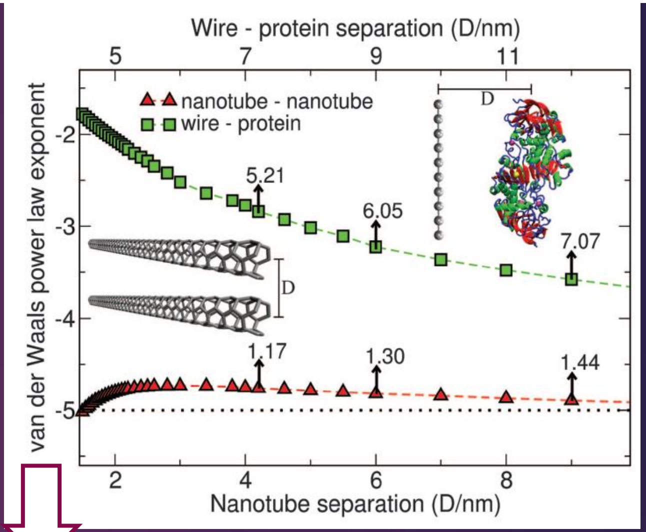
The exchange between **D^{-6}** and **D^{-7}** regimes of the van der Waals dispersion interaction makes microelectromechanical systems Sticky **(dephasing due relativistic signal retardation in the D^{-7} regime).**



CHEMICAL PHYSICS

Wavelike charge density fluctuations and van der Waals interactions at the nanoscale

Alberto Ambrosetti,[1,2] Nicola Ferri,[1] Robert A. DiStasio Jr.,[3*] Alexandre Tkatchenko[1,4*]



Distance dependence of the van der Waals dispersion interaction regime

Langmuir **2008,** *24,* 2274−2276

Superlubricity Using Repulsive van der Waals Forces

Adam A. Feiler,[†,‡] Lennart Bergström,[*,‡,§] and Mark W. Rutland[*,†,‡]

Repulsive version of the van del Waals interaction !

Thus…

As dispersion interaction permeates the whole structure of proteins… it is posible to hyphotesize that…

The Hyphotesis

1.1) When the oscillation of the induced dipoles is **synchronized** an enhanced interacting $\mathbf{D^{-6}}$ regime is triggered and the protein structure start to fold

1.2) The propagation of this regime throughout the molecular structure complete the folding process.

2.1) If a strong enough perturbation is introduced in the cooperative synchronized network a weakened $\mathbf{D^{-7}}$ or even a **repulsive regime** starts to dominate in the molecular protein structure

2.2) This weakened or repulsive regime is associated to the **desynchronization** of the oscillating network and triggers a phase transition that finally unfolds the protein.

So…

Cooperativity is originated by synchronization/desynchronization of the oscillatory phases of van der Waals interaction

PHYSICAL REVIEW B **87**, 144103 (2013)

Quantum Drude oscillator model of atoms and molecules: Many-body polarization and dispersion interactions for atomistic simulation

Andrew P. Jones and Jason Crain

School of Physics, The University of Edinburgh, Mayfield Road, Edinburgh EH9 3JZ, United Kingdom

- Theoretical models indicate that the van der Waals dispersión interation has its origin at the UV range

molecules MDPI

Review

UV-Denaturation Assay to Assess Protein Photostability and Ligand-Binding Interactions Using the High Photon Flux of Diamond B23 Beamline for SRCD

Rohanah Hussain *, Edoardo Longo and Giuliano Siligardi *

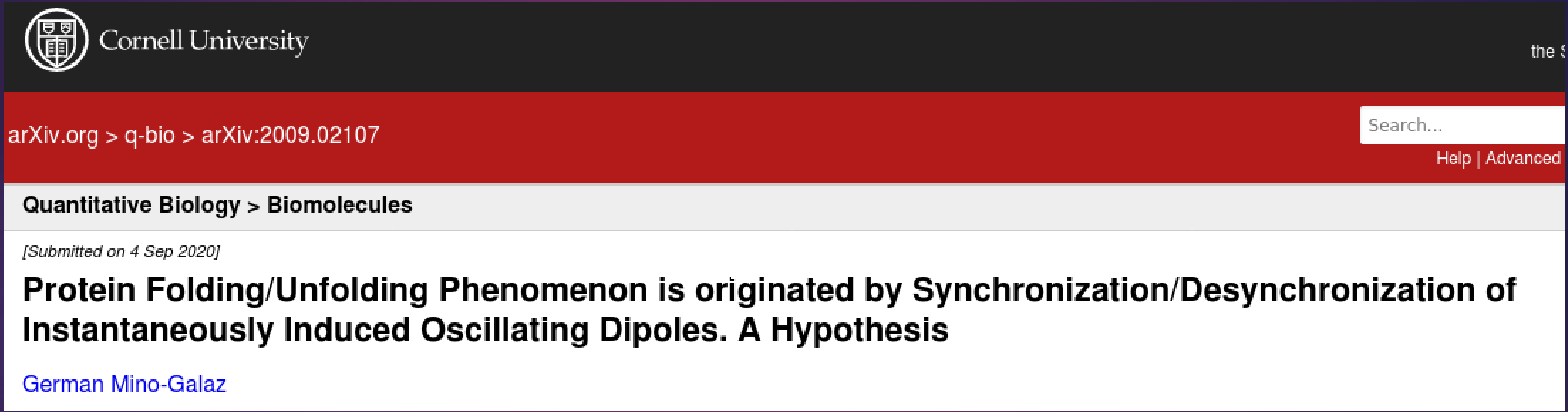
Experimental results shows that UV light denature proteins.

Thus a mechanism a of modulable frecuency of oscillatory dipoles may underpin
Protein folding/unfolding phenomenology

A general mechanism is proposed in which two opposed operative actions -synchronization/desynchronization- acts to modulate the state -folded/unfolded- of the same object, a protein.

Further information

https://arxiv.org/abs/2009.02107


Cornell University

the S

arXiv.org > q-bio > arXiv:2009.02107

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[Submitted on 4 Sep 2020]

Protein Folding/Unfolding Phenomenon is originated by Synchronization/Desynchronization of Instantaneously Induced Oscillating Dipoles. A Hypothesis

German Mino-Galaz

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