



KEMIJSKI INŠTITUT

Vabilo na Forum40 / Invitation to the Forum40

**Dr. Petra Papež**

Theory department

Četrtek / Thursday, 16. 4. 2026 ob / at 13:00

Velika predavalnica Kemijskega inštituta / Great Lecture Hall

WEBEX

<https://ki-ljubljana.webex.com/ki-ljubljana/j.php?MTID=m8ad688fb936bfad8195c9bb370fe2f21>

Meeting number: 2781 260 6476

Meeting password: i3FuQJJk2Q9

## Protein vibrational and rotational dynamics unveiled using OBMD method as a virtual ultrasound machine and rheometer

Proteins are building blocks of living organisms, and their 3D structure encodes motions that determine their activity. Protein function and activity can be impaired by mechanical stress (e.g., shear flow and mechanical pressure waves), and the open-boundary molecular dynamics (OBMD) method represents a promising computational tool to investigate such effects.

By employing the OBMD method, we explore how hydrodynamic shear flow and acoustic excitations influence the internal, rotational, and conformational dynamics of a protein. Our findings demonstrate that extraordinarily high shear rates must be applied to observe protein unfolding and that acoustic waves enhance its internal dynamics.



Vljudno vabljeni / Kindly invited