

ELECTRONIC SUPPLEMENTARY INFORMATION

Microscopic modelling of nematic elastic constants beyond Straley theory

Davide Revignas and Alberta Ferrarini*

Università di Padova

Dipartimento di Scienze Chimiche, via Marzolo 1, 35131 Padova, Italy

*alberta.ferrarini@unipd.it

Table of Contents

1	Deformations and model particles	2
2	Ideal and excess contributions to Frank elastic constants and plots of ODFs	3
2.1	Rod	3
2.2	Bent Rod	5

1 Deformations and model particles

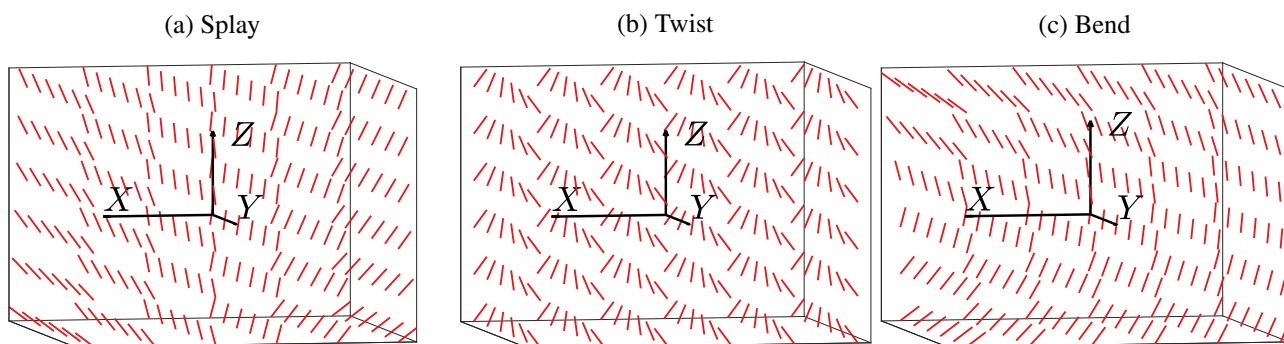


Figure S 1: Sketch of the director field (red) in presence of the three deformations defined in Eqs. (11-12) of the main text. $(OXYZ)$ is the laboratory reference frame.

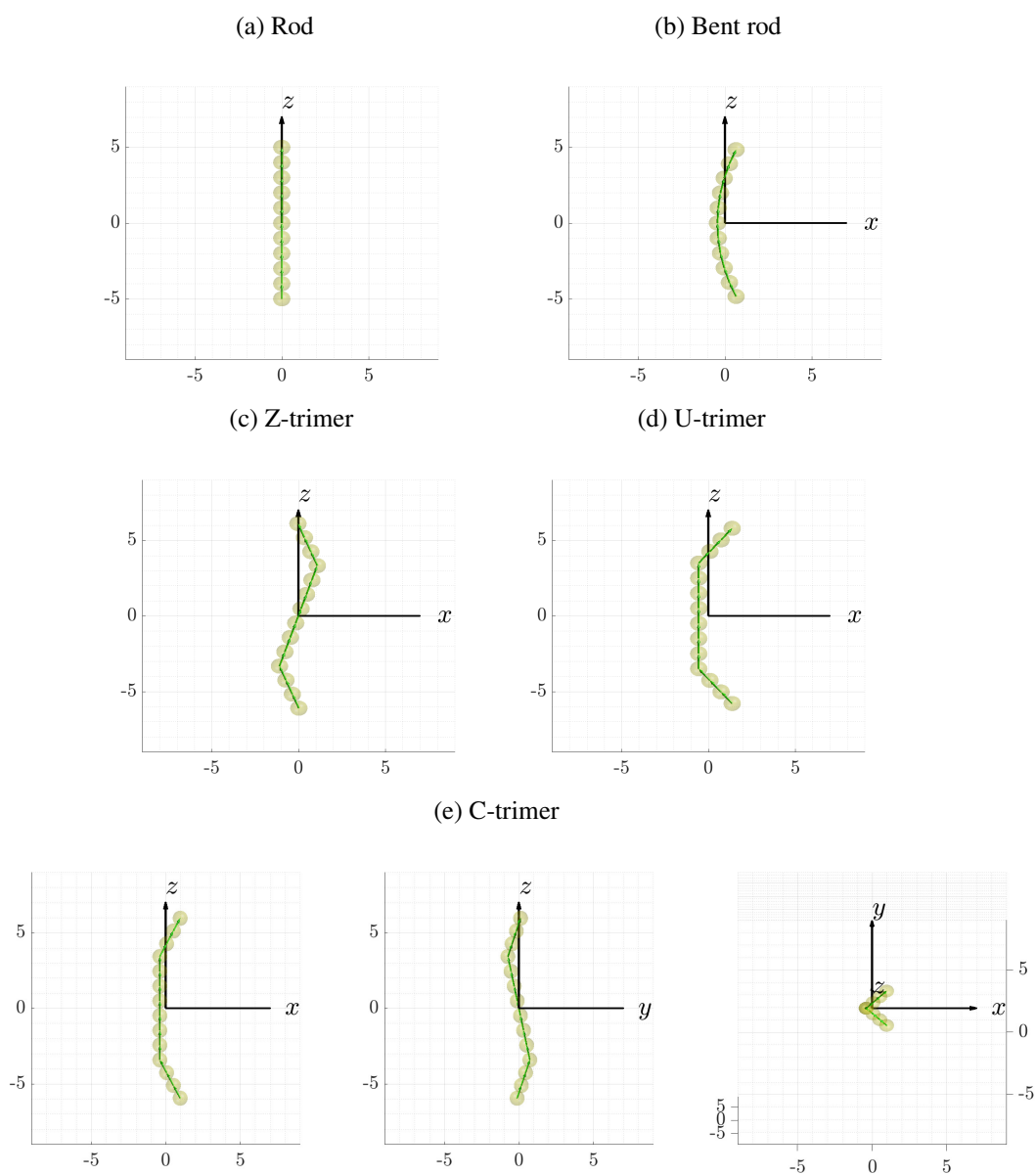


Figure S 2: Sketches of the particles studied in the present work.

2 Ideal and excess contributions to Frank elastic constants and plots of ODFs

2.1 Rod

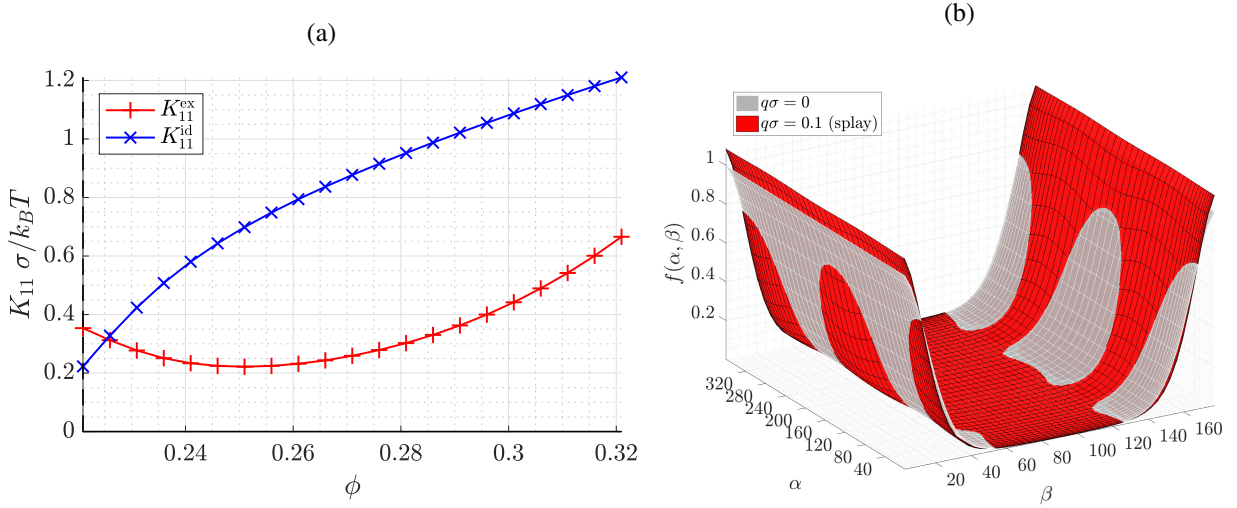


Figure S 3: (a) Contributions to the splay elastic constant, K_{11}^{id} and K_{11}^{ex} , for straight rods, as functions of the packing fraction ϕ . (b) ODF of rods in the uniform nematic phase (gray) and in the presence of a splay deformation (red), as defined in Eqs. (11-12) of the main text. Calculations with orienting strength parameter $a = 0.7$ and deformation wavenumber $q\sigma = 0.1$.

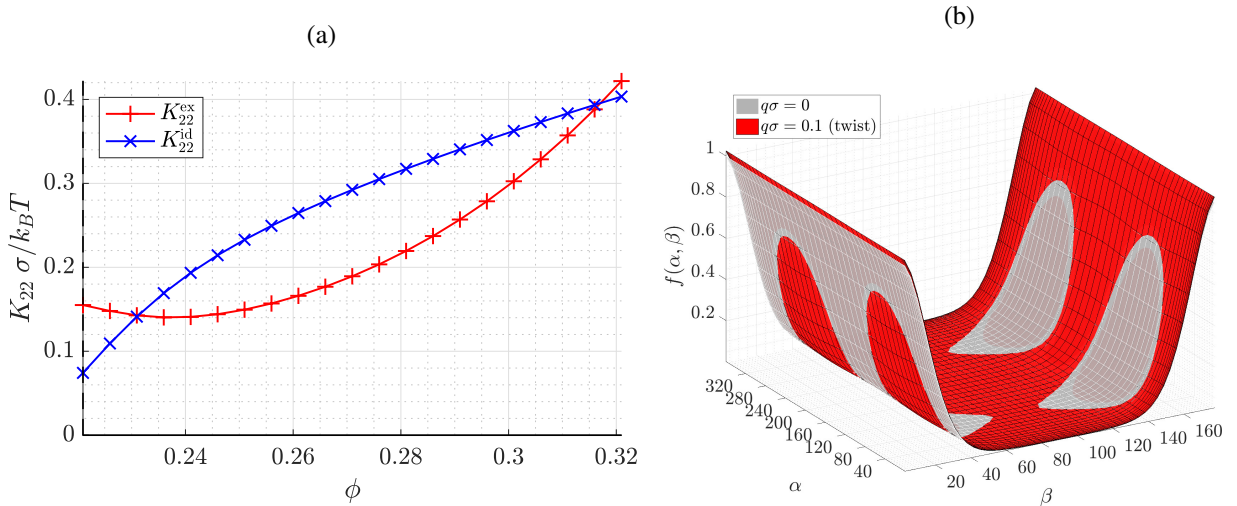


Figure S 4: (a) Contributions to the twist elastic constant, K_{22}^{id} and K_{22}^{ex} , for straight rods, as functions of the packing fraction ϕ . (b) ODF of rods in the uniform nematic phase (gray) and in the presence of a twist deformation (red), as defined in Eqs. (11-12) of the main text. Calculations with orienting strength parameter $a = 0.7$ and deformation wavenumber $q\sigma = 0.1$.

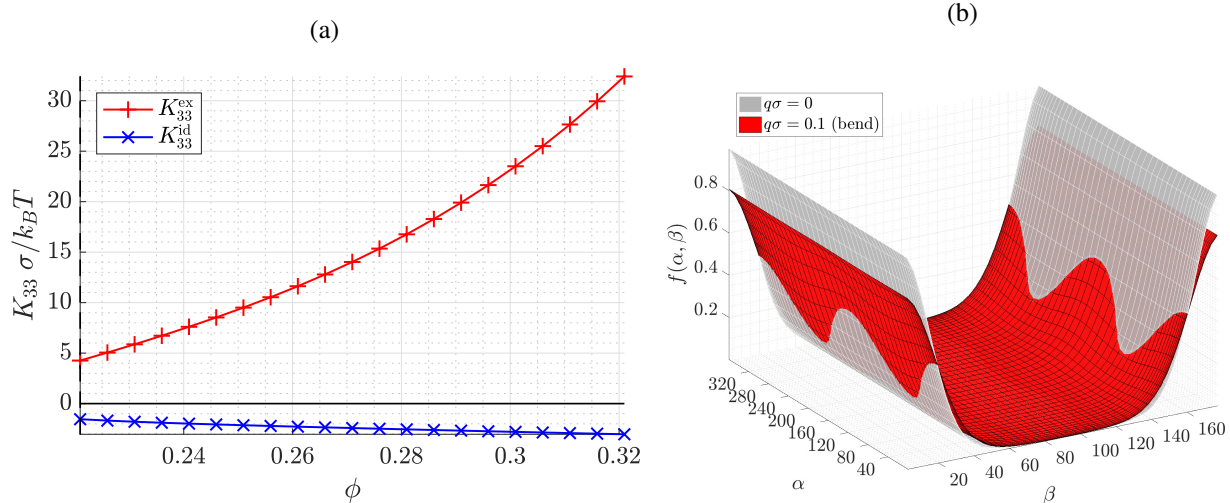
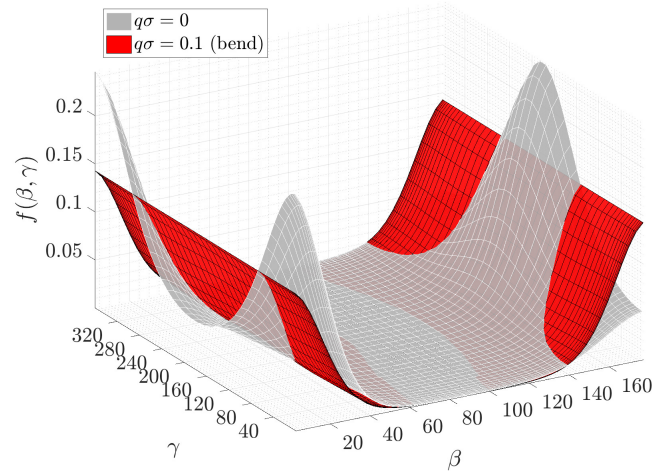


Figure S 5: (a) Contributions to the bend elastic constant, K_{33}^{id} and K_{33}^{ex} , for straight rods, as functions of the packing fraction ϕ . (b) ODF of rods in the uniform nematic phase (gray) and in the presence of a bend deformation (red), as defined in Eqs. (11-12) of the main text. Calculations with orienting strength parameter $a = 0.7$ and deformation wavenumber $q\sigma = 0.1$.

2.2 Bent Rod

(a) ODF plot ($\alpha = 0^\circ$) for bent rods.



(b)

(c)

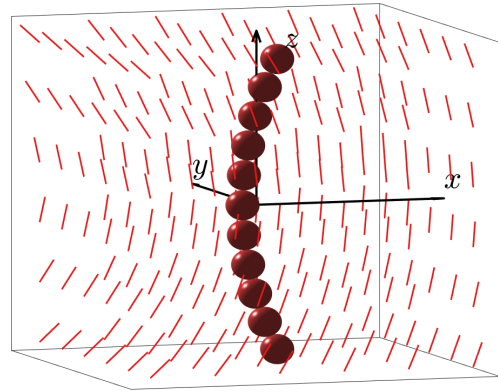
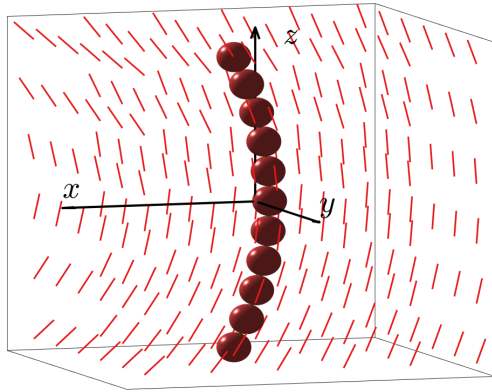


Figure S 6: (a) ODF of bent rods in the uniform nematic phase (gray) and in the presence of a bend deformation (red), as defined in Eqs. (11-12) of the main text. Calculations with orienting strength parameter $a = 0.7$, deformation wavenumber $q\sigma = 0.1$ and $\alpha = 0^\circ$. The angles β and γ describe rotations around the molecular axes y and z , respectively. (b) Sketch of a bent rod immersed in a bent director field (red segments), in the orientation defined by the Euler angles $\alpha = 0^\circ, \beta = 0^\circ, \gamma = 0^\circ$ (particle and distortion concavity in accordance), and (c) $\alpha = 0^\circ, \beta = 0^\circ, \gamma = 180^\circ$ (particle and distortion concavity in opposition).

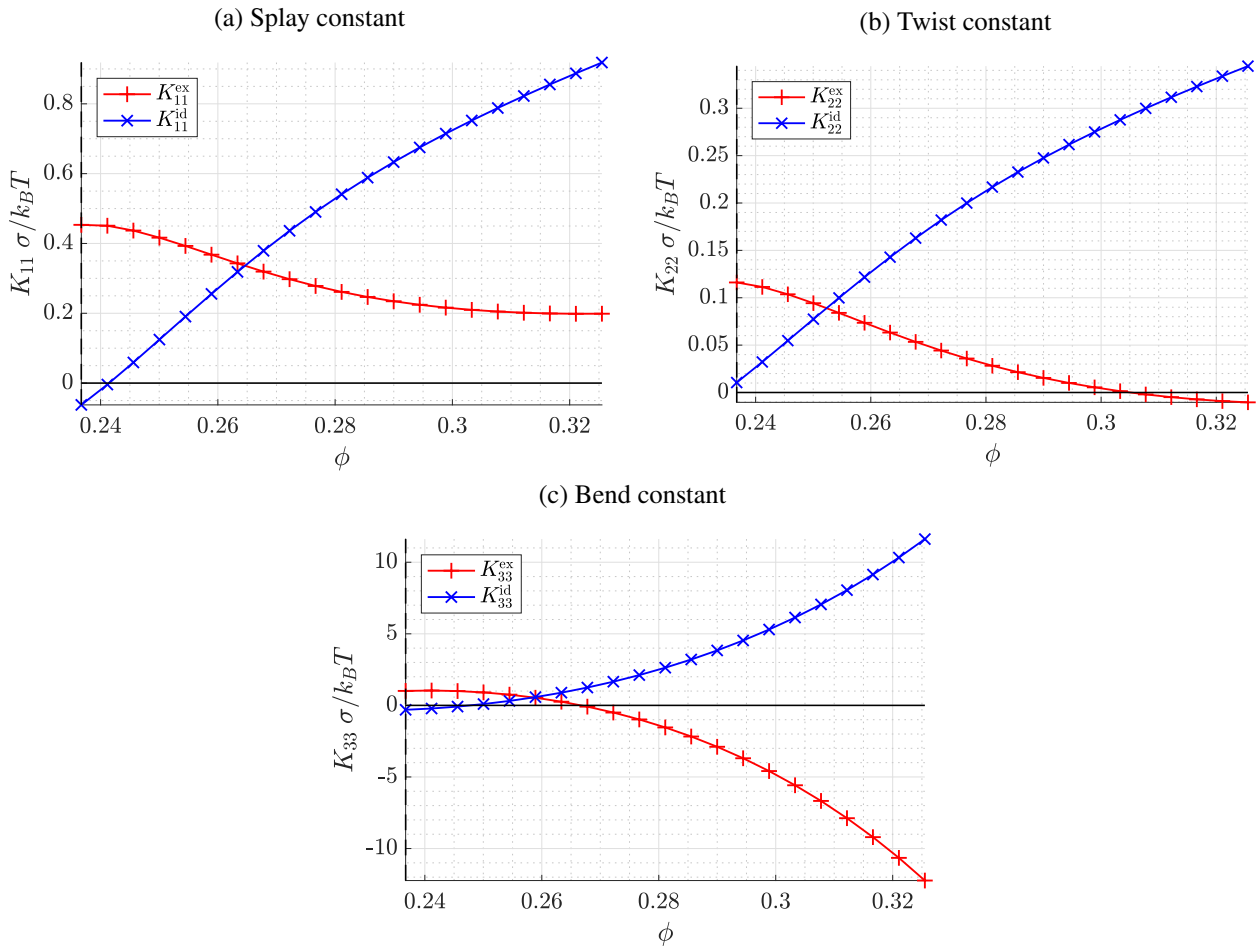


Figure S 7: Ideal and excess contributions to elastic constants for bent rod particles, as functions of the packing fraction ϕ .