

Defects and shell stability under external pressure

Duanduan Wan¹, Mark Bowick¹, Rastko Sknepnek²

1. Department of Physics, Syracuse University, Syracuse NY 13244, USA

2. Division of Physics and Division of Computational Biology, University of Dundee, Dundee DD1 4HN, UK

For any triangulation of a sphere:

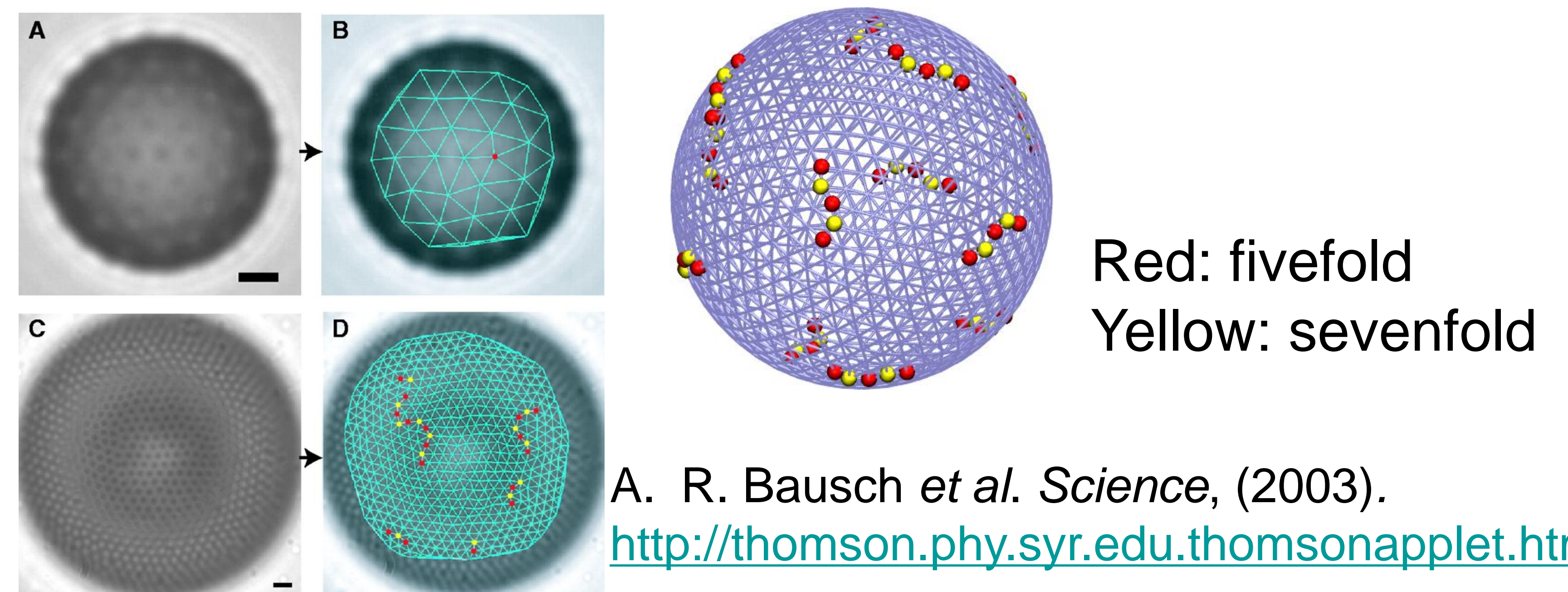
$$\sum_i q_i = \sum_i (6 - c_i) = 6\chi = 12$$

If limited to $q = \pm 1$ charges:

Minimal set of defects:
Twelve +1 disclinations

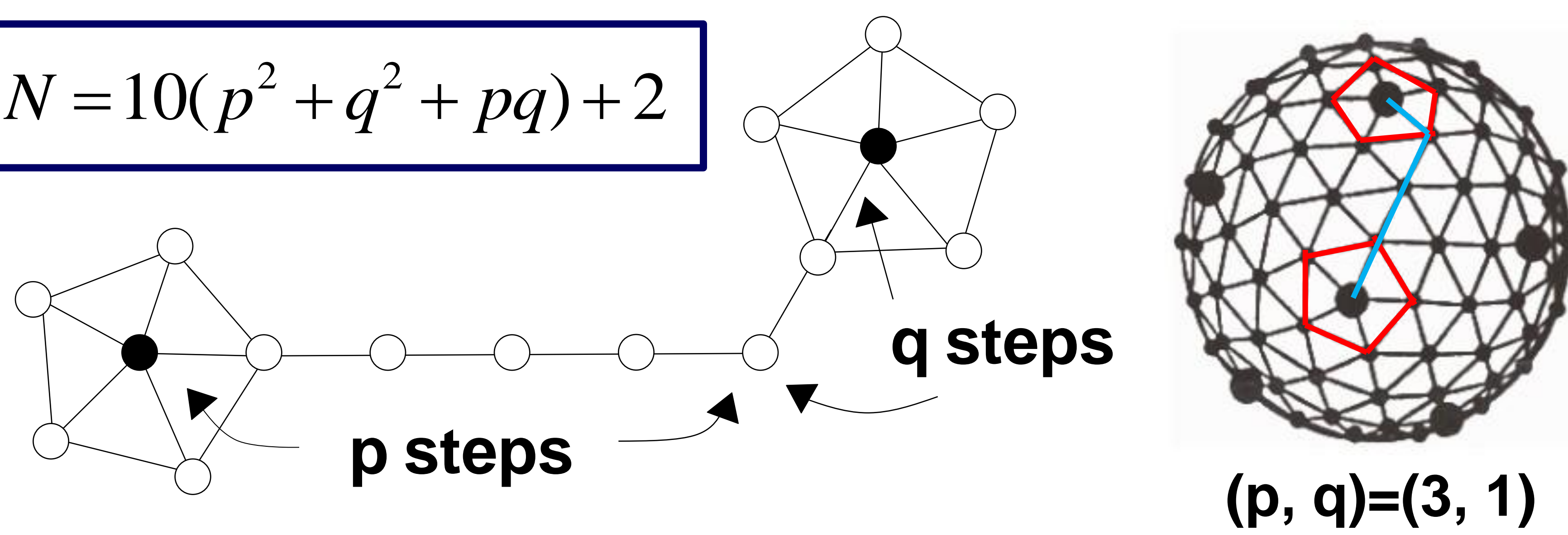
Extended defect arrays:
Grain boundary "scars"

Grain boundary scars



Icosadeltahedral shells and Caspar-Klug notations

$$N = 10(p^2 + q^2 + pq) + 2$$



D. L. D. Caspar and A. Klug. *Cold Spring Harb. Symp. Quant. Biol.*, (1962).
J. Lidmar, L. Mirny and D. R. Nelson. *PRE*, (2003).

Energy

$$F_{tot} = F_{stretching} + F_{bending} + PV$$

Continuum elasticity:

$$F_s = \frac{1}{2} \int dS (2\mu u_{ij}^2 + \lambda u_{kk}^2)$$

$$F_b = \frac{1}{2} \int dS (2\kappa H^2 + \kappa_G K)$$

Discretized version:

$$F_s = \frac{\epsilon}{2} \sum_{\langle ij \rangle} (|\mathbf{r}_i - \mathbf{r}_j| - a)^2$$

$$F_b = \frac{\tilde{\kappa}}{2} \sum_{\langle IJ \rangle} (\hat{\mathbf{n}}_I - \hat{\mathbf{n}}_J)^2$$

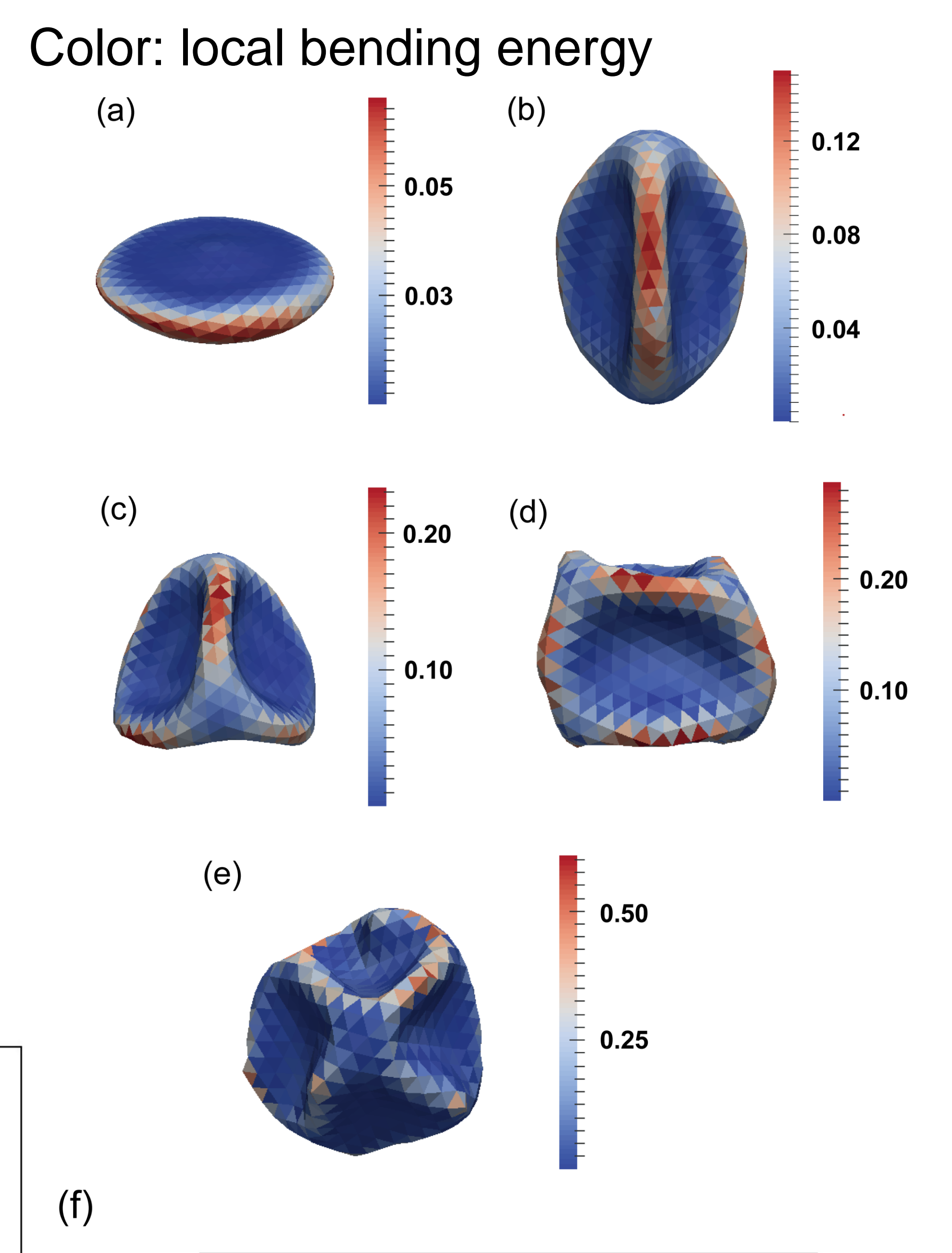
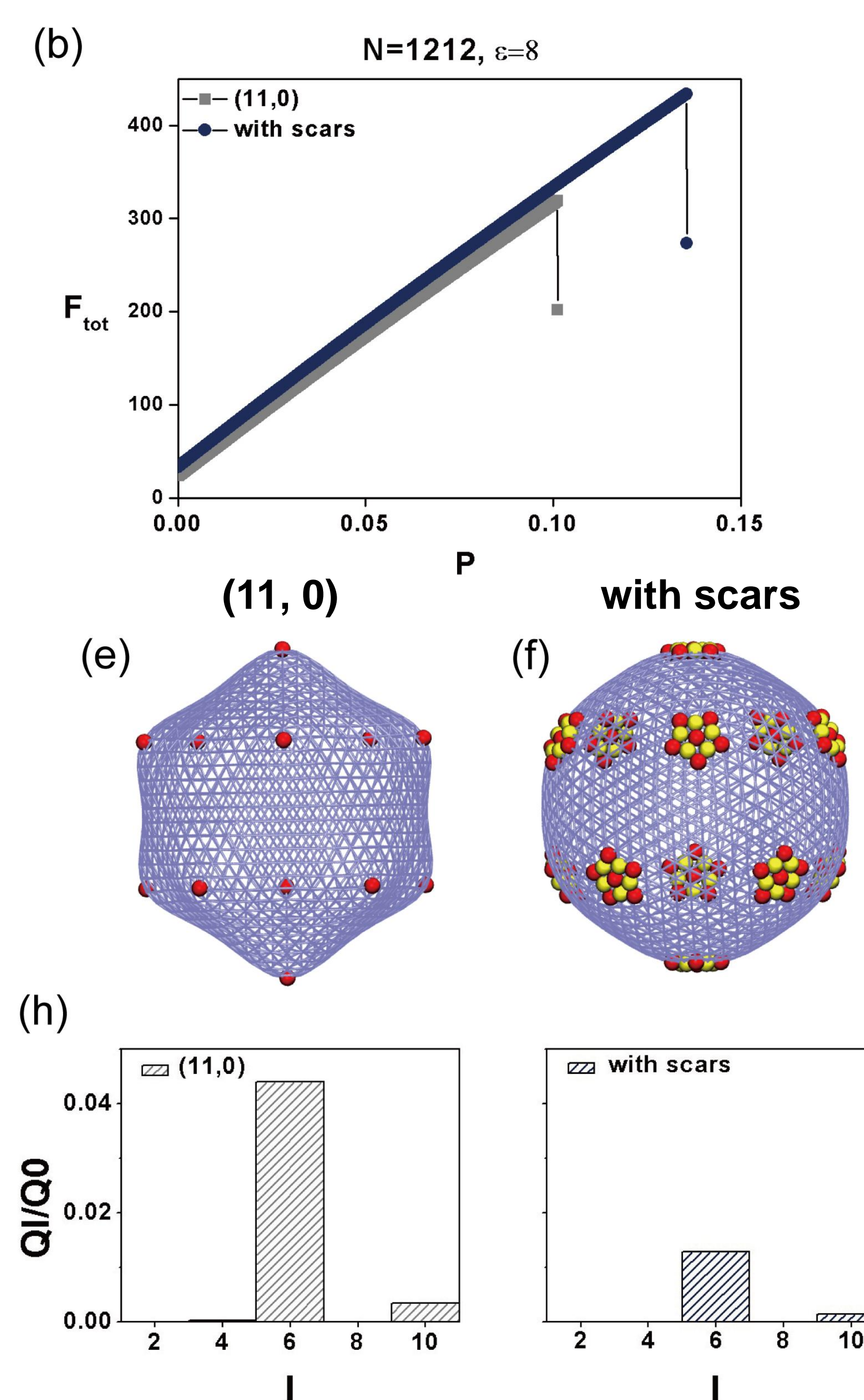
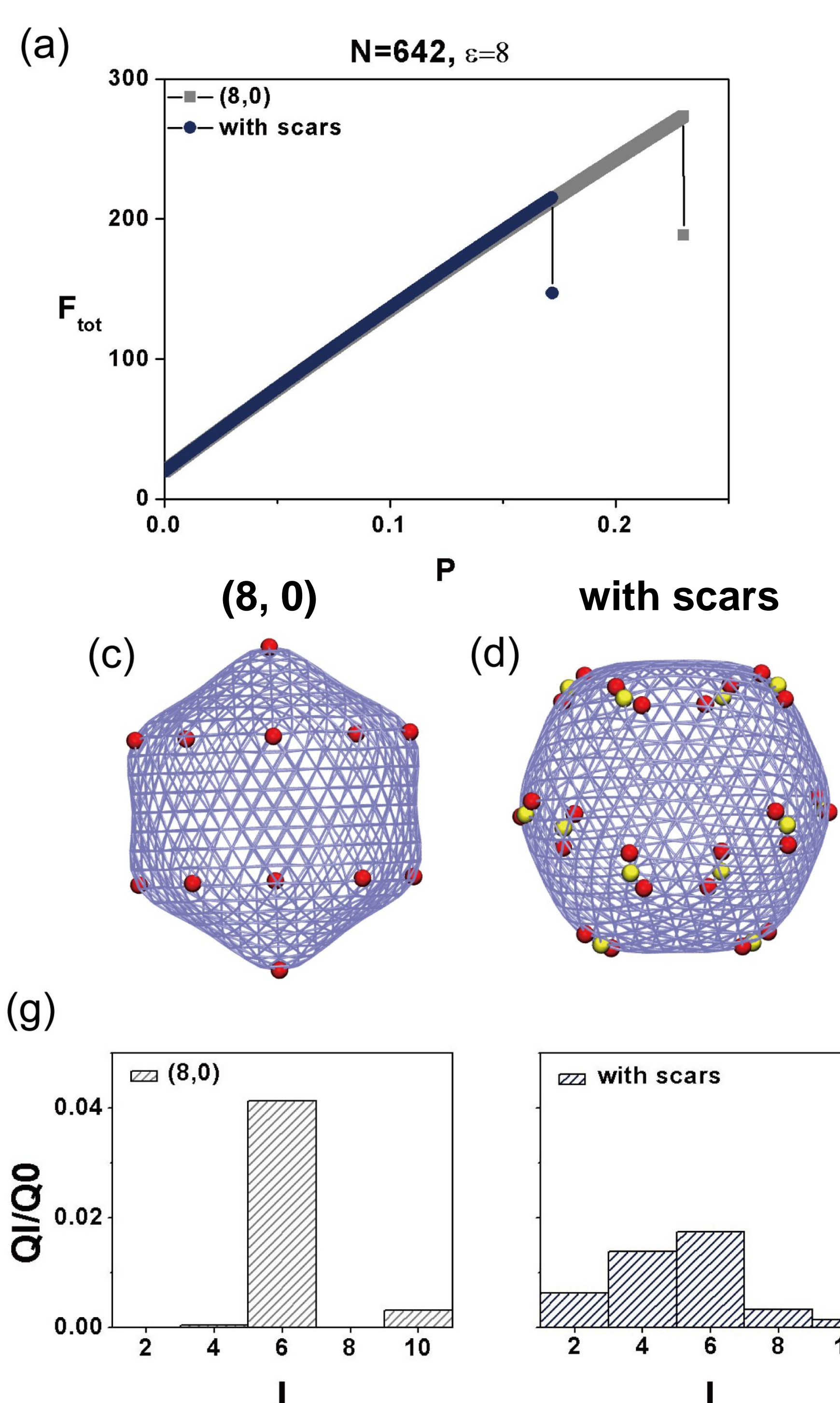
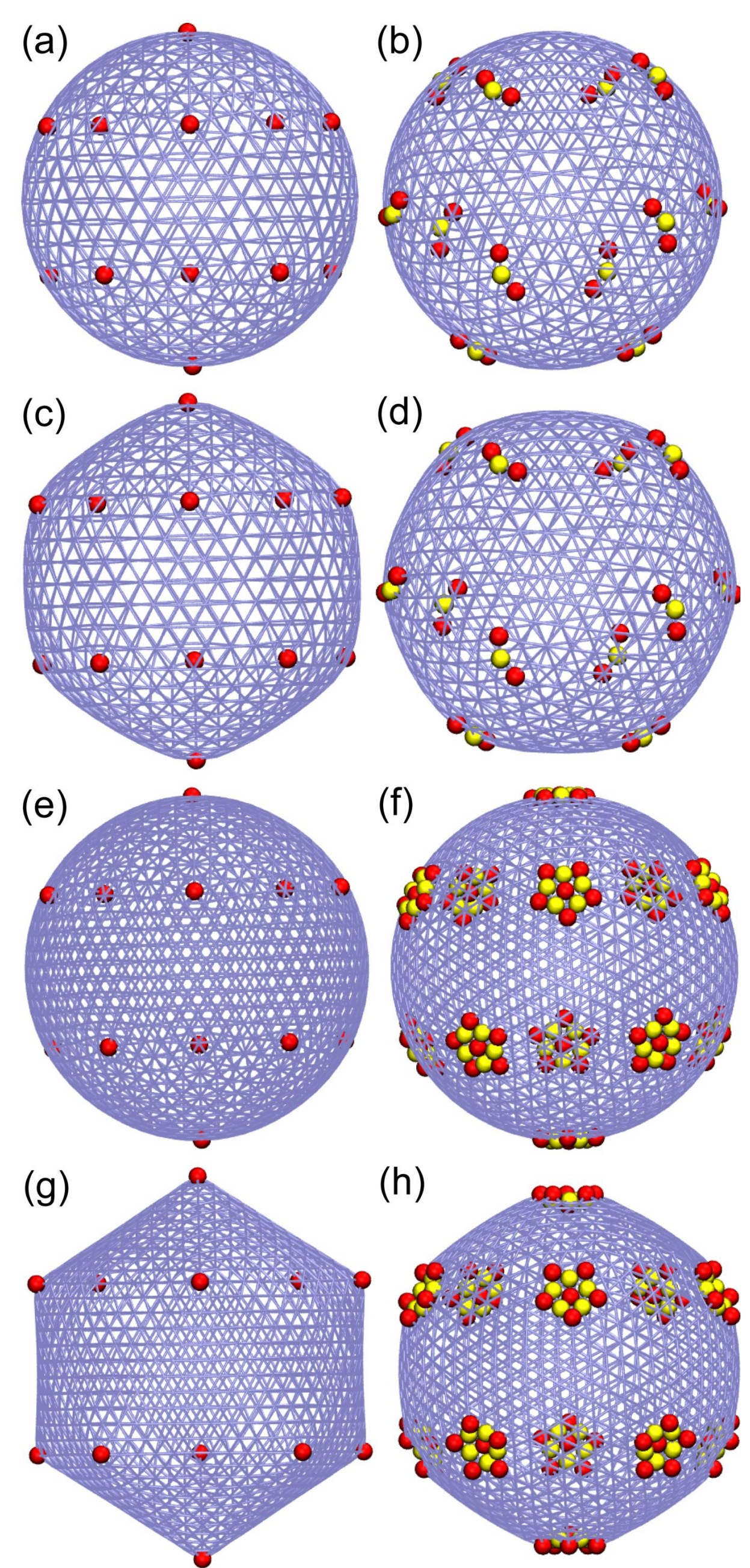
L. D. Landau and E. M. Lifshitz. *Theory of Elasticity*, 3rd edition, (2003).

Comparison of shells without and with scars in (8,0) and (11,0) cases

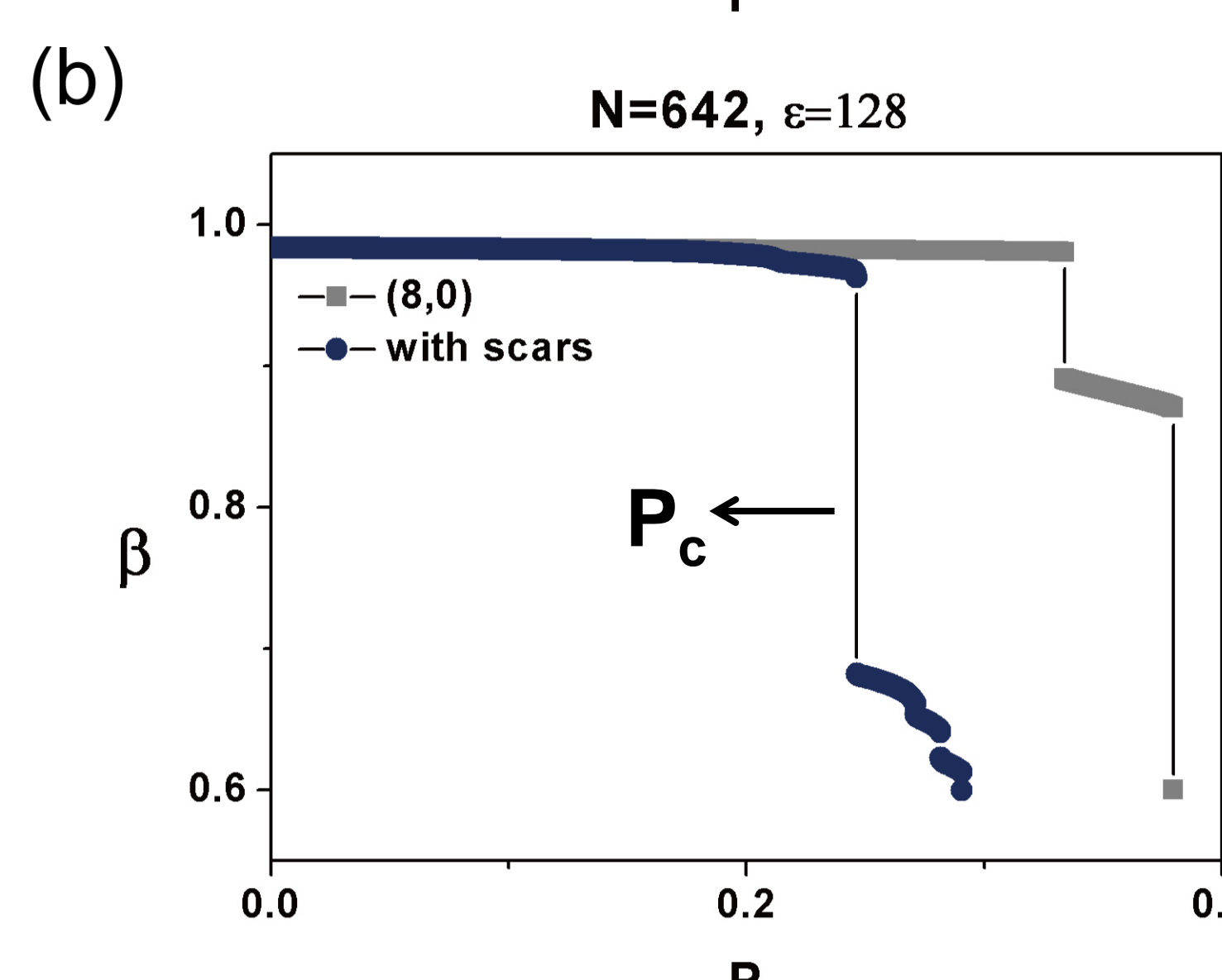
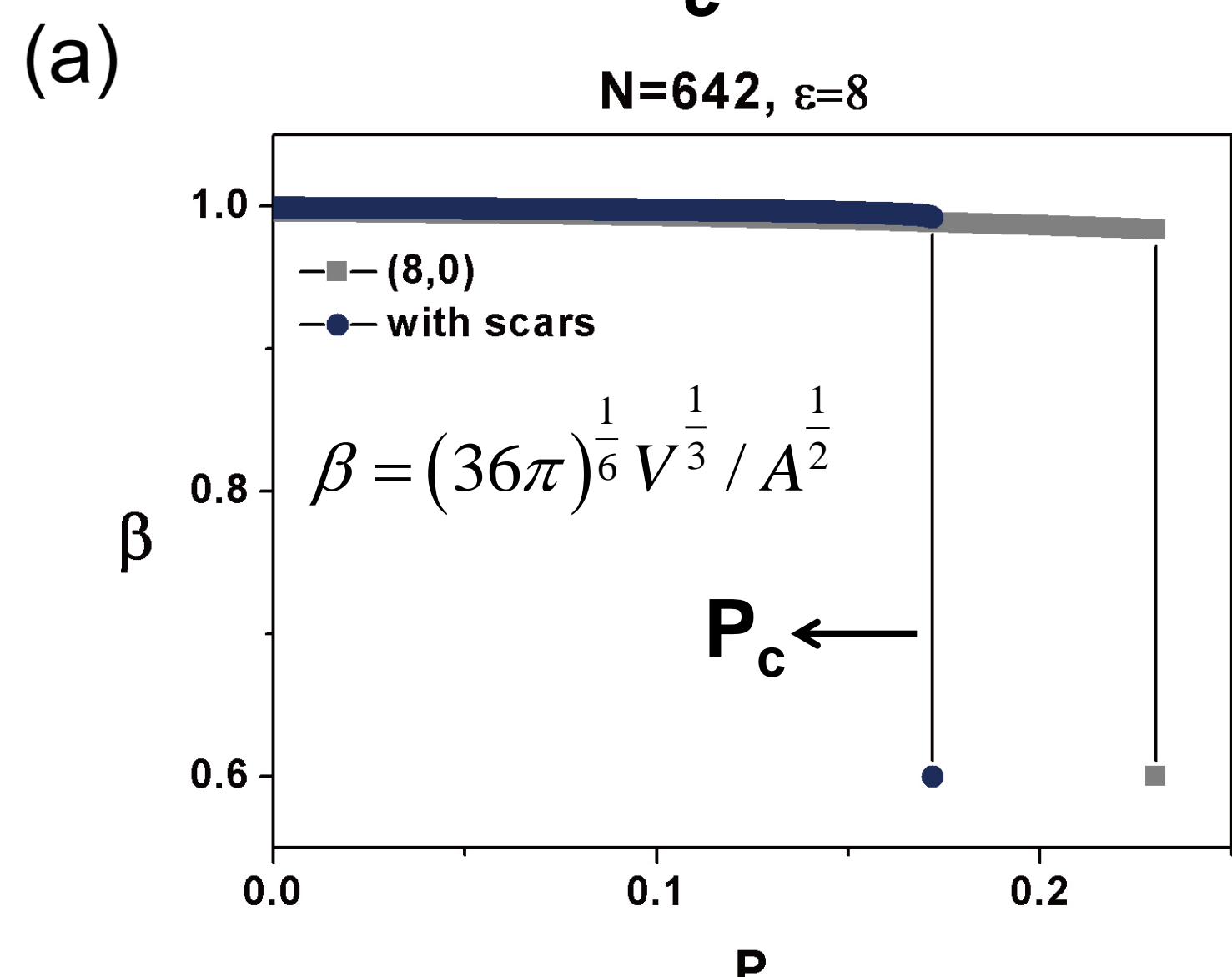
In the absence of pressure

Configurations before collapse

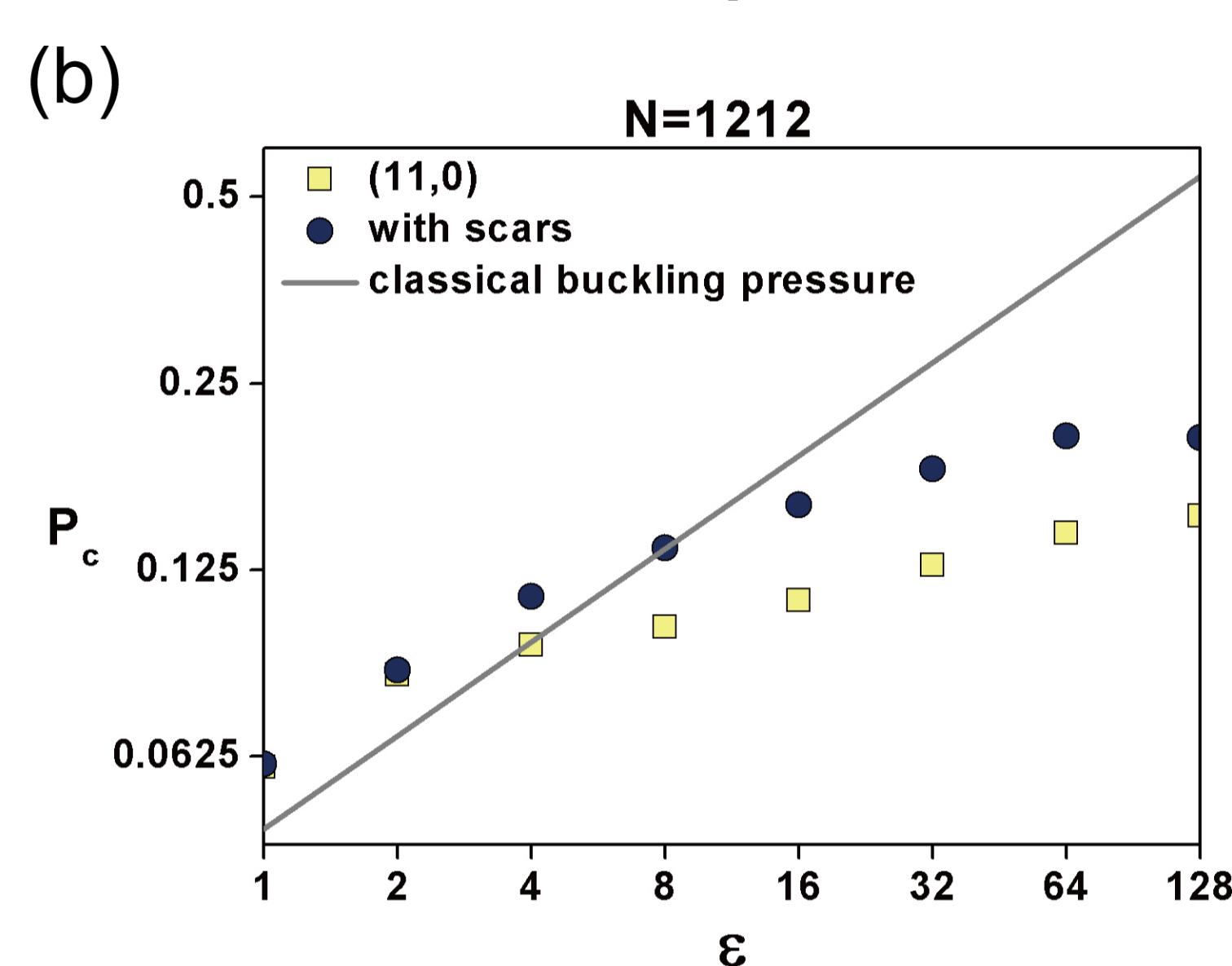
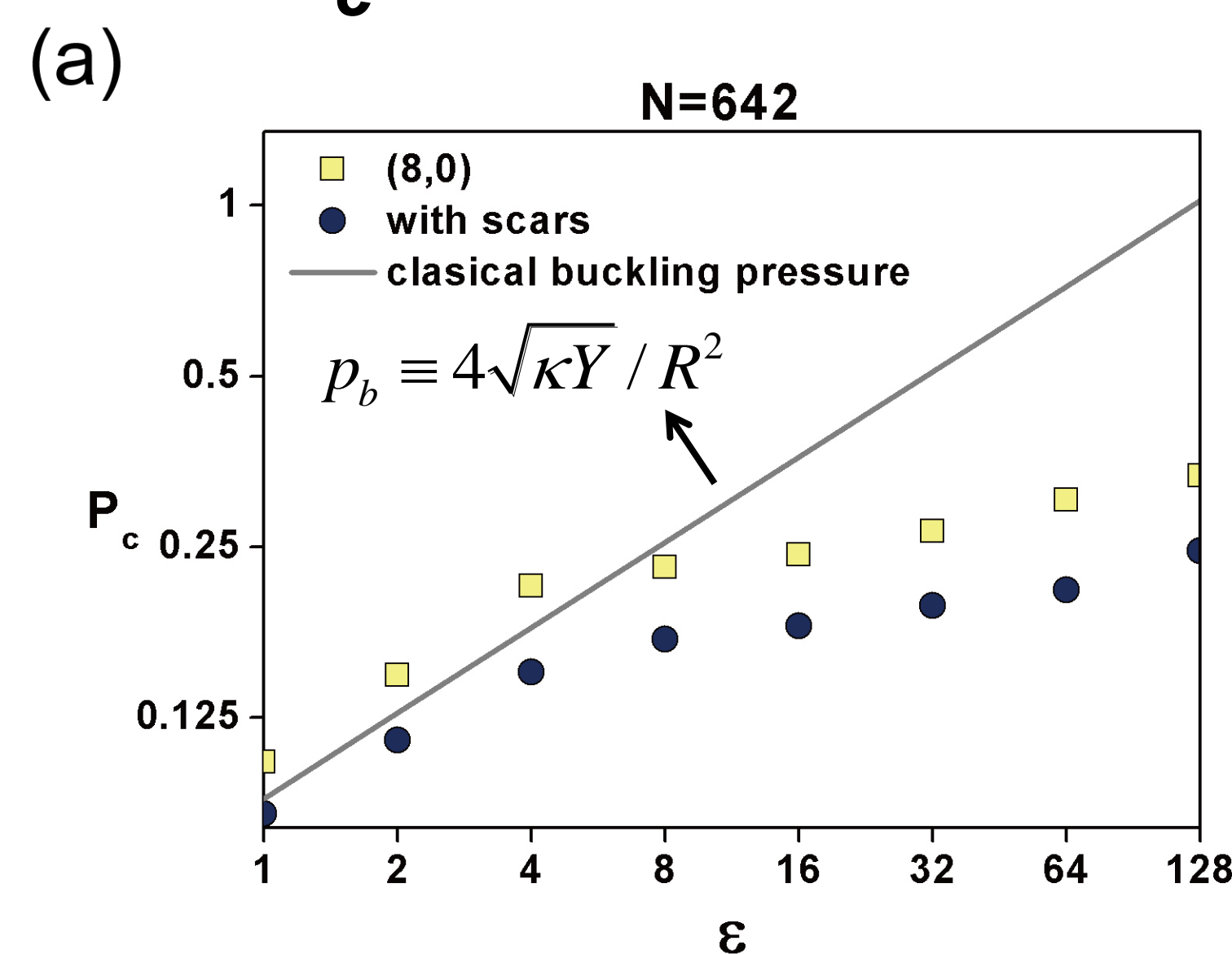
Configurations during collapse



Define P_c



P_c behavior



$l=6, 10$ components are a signal of icosahedral symmetry.

Conclusions

Mechanisms affect the critical pressure:
(1) the preservation of icosahedral symmetry
(2) the area occupied by scars

Acknowledgments

This research was supported by the Soft Matter Program of Syracuse University.