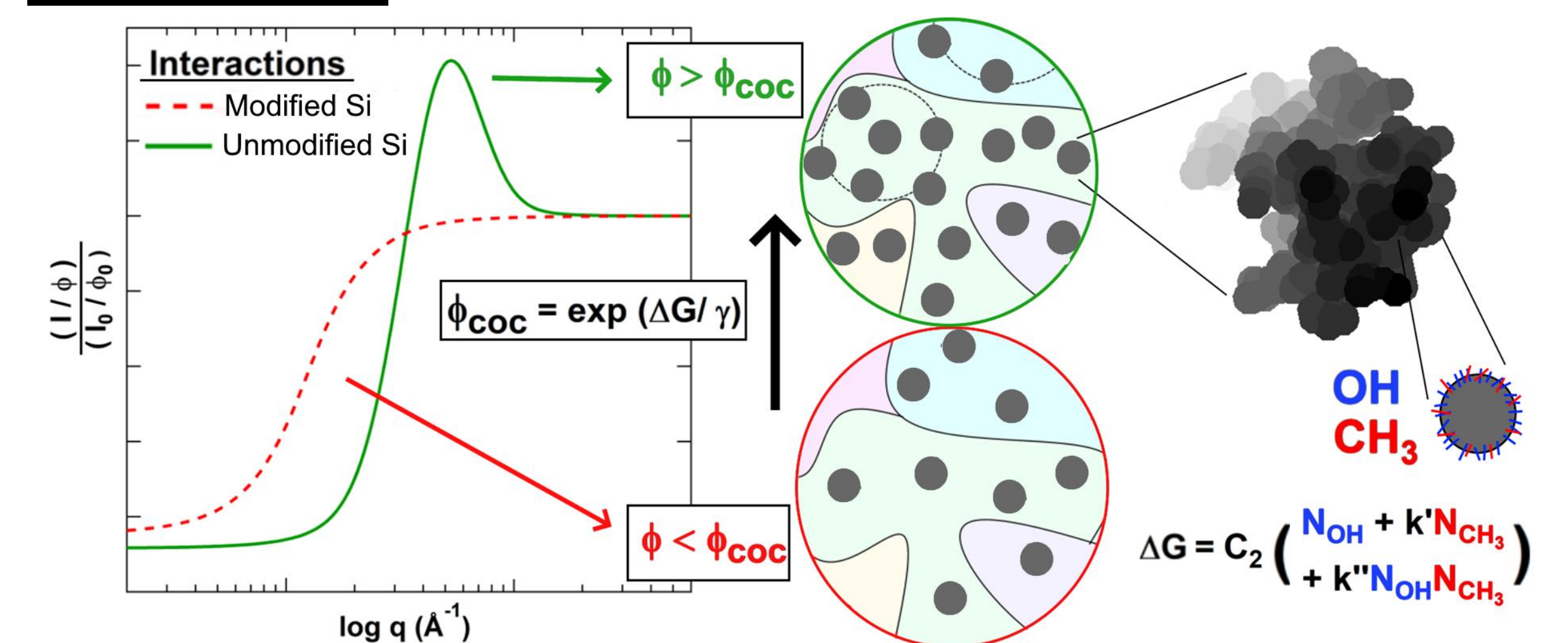


Compatibility/Incompatibility in surface-modified, aggregated, precipitated silica nanocomposites

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Overview



Model

Surface interactions:

(a) Weak (Random Phase Approximation^{1,2})

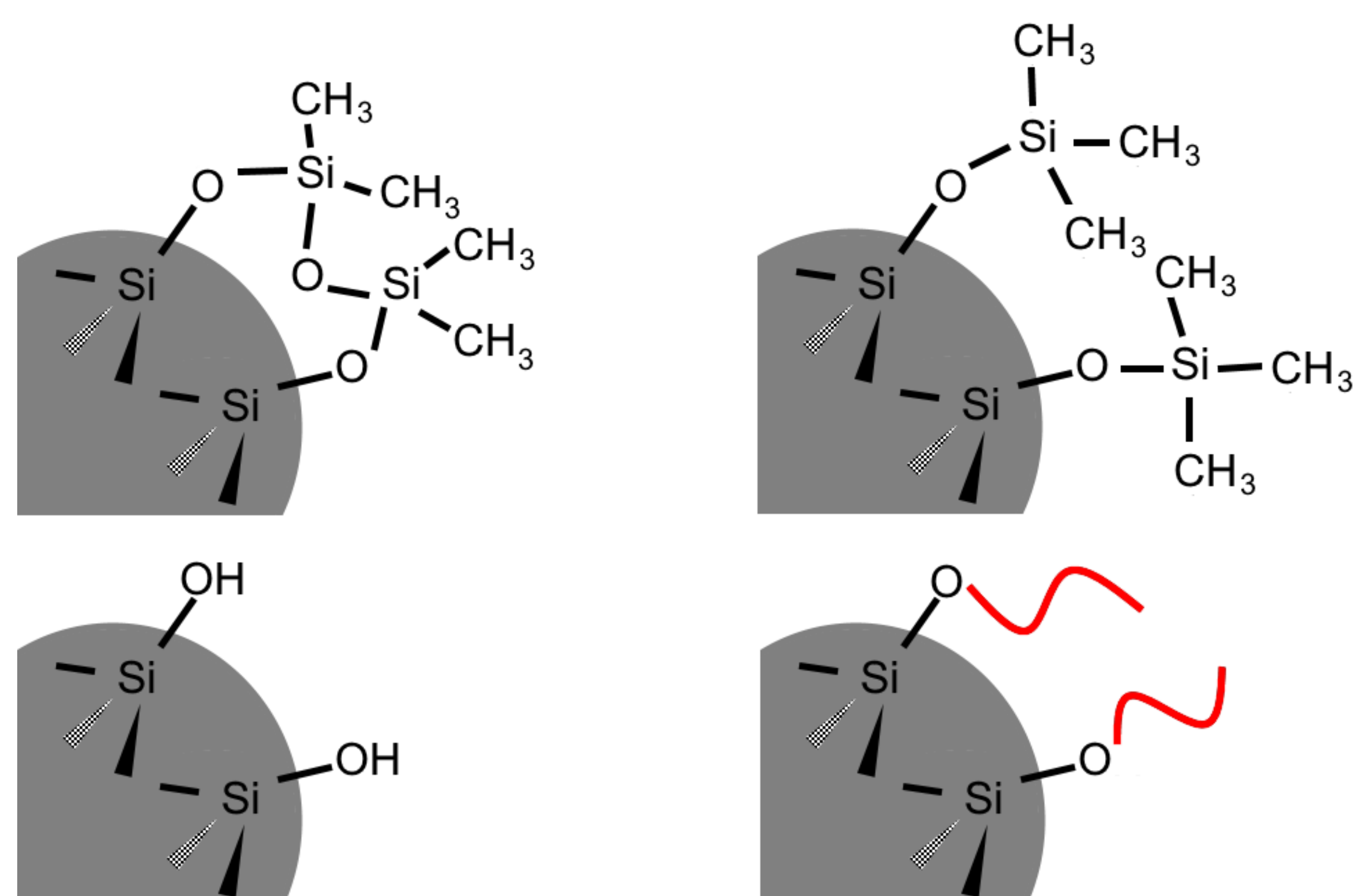
$$S(q) = \frac{1}{1 + \phi v \left(I_o(q) / \phi_0 \right)}$$

(a) Strong (modified Born-Green approach³)

$$S(q, \xi) = \int_0^\infty P(\xi) \left[\frac{1}{1 + p\theta(q, \xi)} \right] d\xi$$

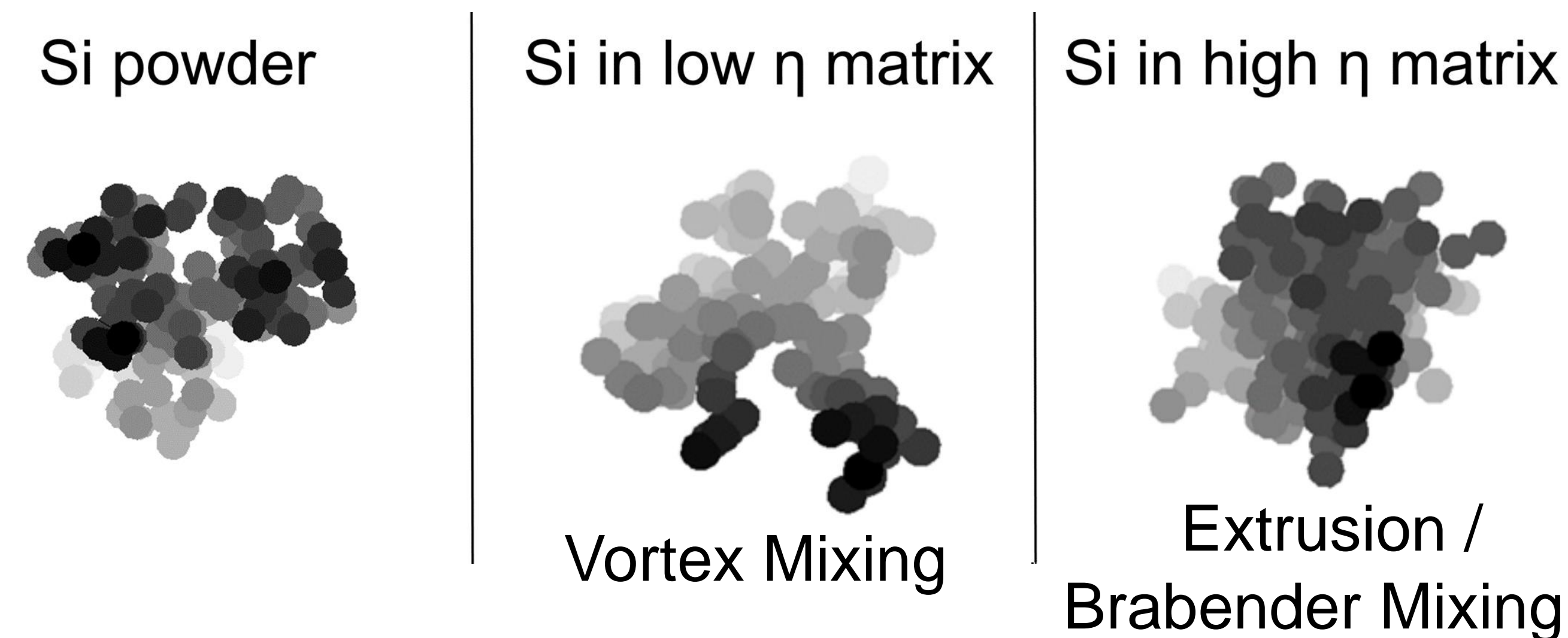
Methods

Commercial SBR (80M.U.), PS (*MW*- 125K g/mol) & CH₃-terminated PDMS (*MW*- 500 g/mol) mixed with fumed silica (unmodified, surface modified, grafted)



Aggregate Morphology

Structural information from Unified fit⁵ (dilute filler) & resulting simulated aggregate⁶



Adapted from Rishi, K.; Pallerla, A.; Beaucage, G.; Tang, A. Dispersion of surface-modified, aggregated, fumed silica in polymer nanocomposites. This article has been accepted by *J. Appl. Physics*. After it is published, it will be found at [Link](#). Copyright 2020 American Institute of Physics

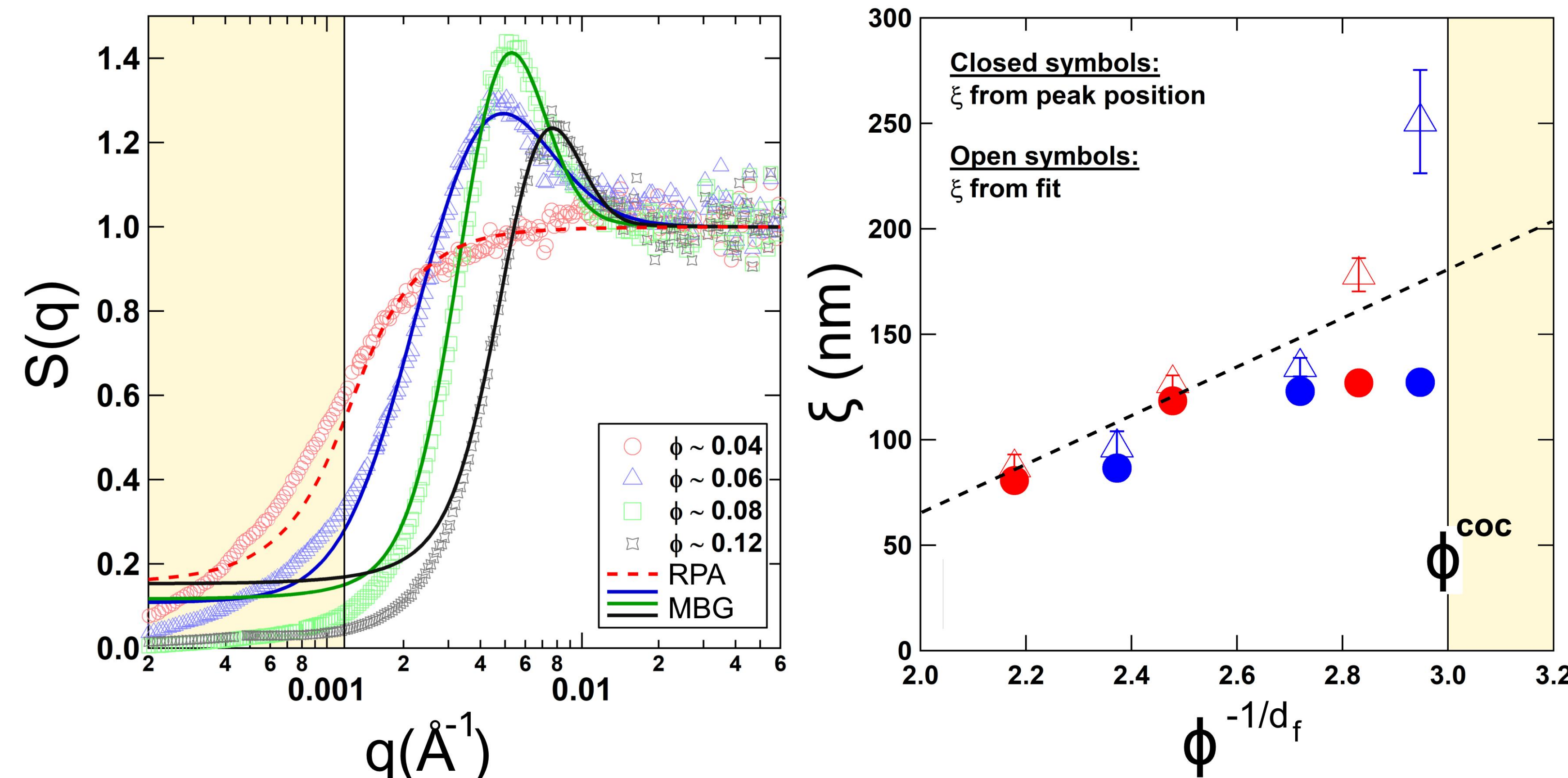
Critical Ordering Concentration (Unmodified Si)

$$\lambda_D \propto \kappa^{1/2}$$

$$\kappa_{SBR} > \kappa_{PS} \sim \kappa_{PDMS}$$

Discovery⁴:
Ordering criterion:
 $\xi < \lambda_D$

Unmodified Si in SBR



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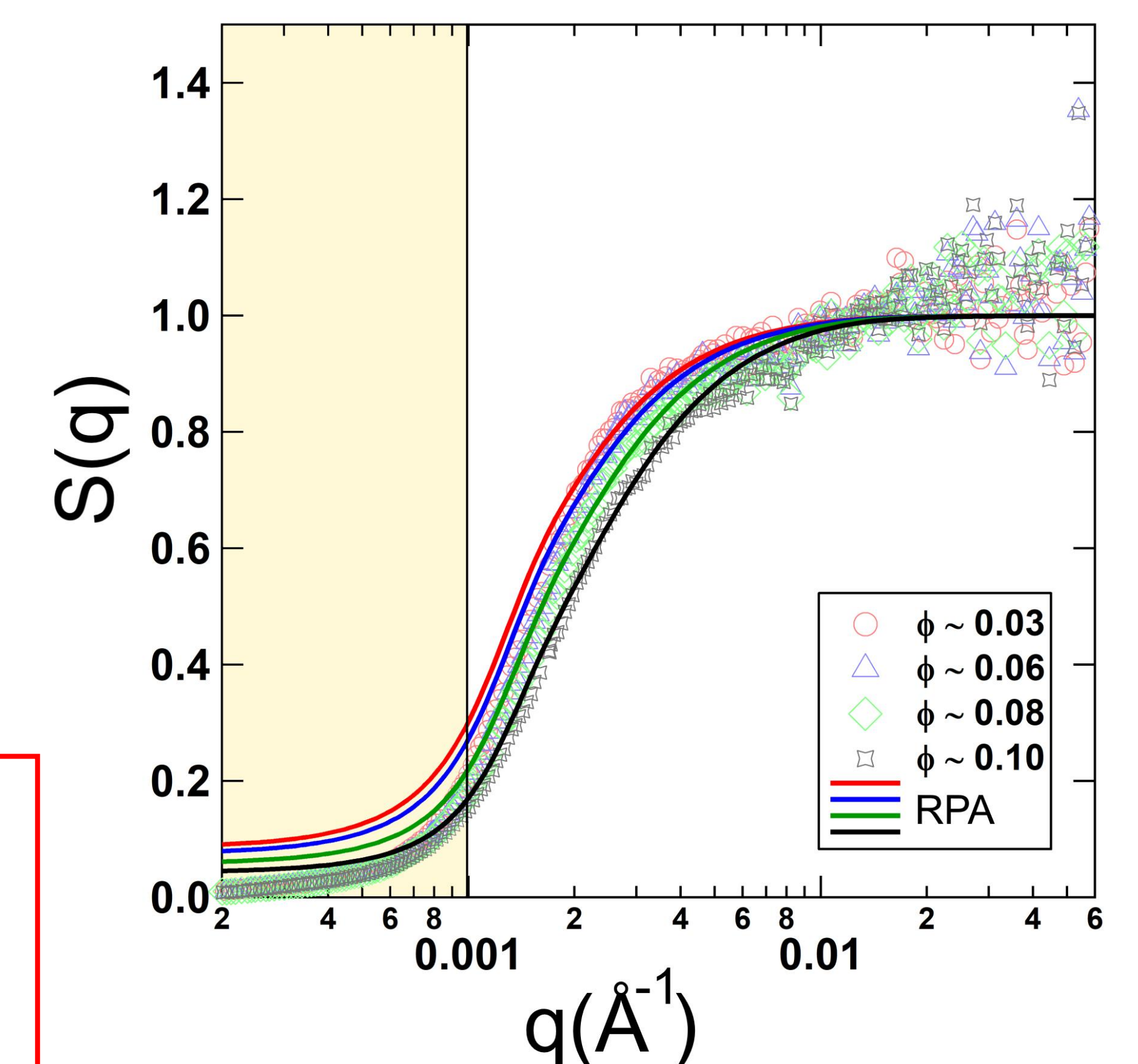
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Mean field (Modified Si)

$$v \propto \frac{p}{\phi} \propto A_2$$

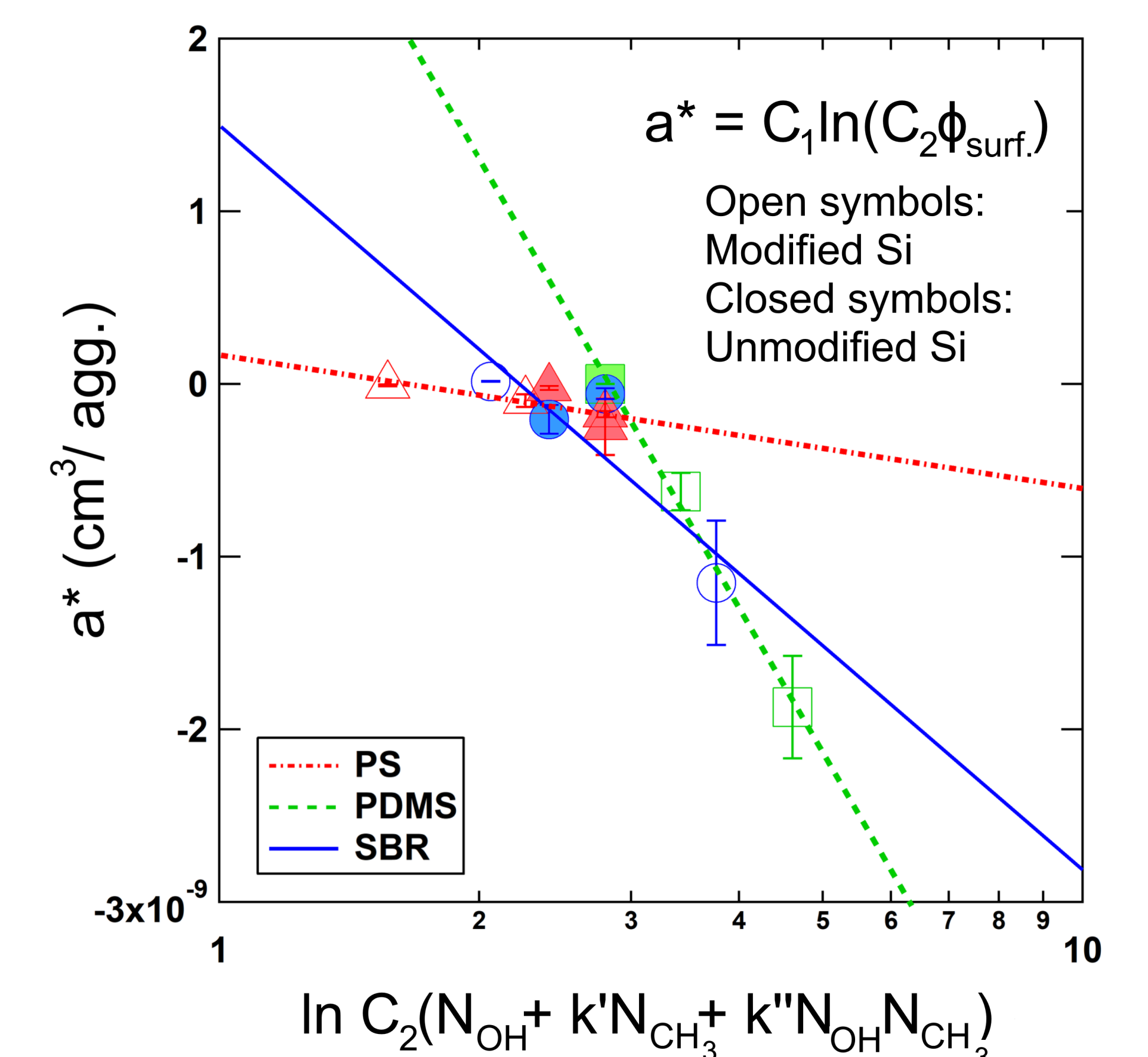
$$A_2 \propto b^* - (a^*/\gamma)$$

Modified Si in SBR



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Interaction potential / Energy of aggregation



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