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Dispersion of Mixed Brush Gold Nanorods in Polymer Matrices
ROBERT FERRIER, JASON KOSKI, ROBERT RIGGLEMAN, RUSSELL COMPOSTO, University of Pennsylvania — In this work we investigate, both experimentally and through hybrid particle/self-consistent field theoretic (hSCFT) calculations, the dispersion state of gold nanorods (AuNRs) grafted with homopolymer, bidispersed, or mixed polymer brushes. AuNRs are grafted with 11.5 kg/mol PS (HNRs), 11.5 kg/mol PS and 5.3 kg/mol PS (BNRs), or 11.5 kg/mol PS and 5 kg/mol poly(methyl methacrylate) (PMMA) (MBNRs) and cast in PS or PMMA films consisting of short to very long chains compared to the grafted brush. We further investigated the MBNR systems by varying the length of the PS brush. Overall, we find that the MBNRs dispersed markedly better than the other brush types (HNRs or BNRs) in PS matrices. We utilize hSCFT calculations, in particular potential of mean force (PMF) and brush profile calculations, to elucidate the thermodynamics of these systems. The PMFs and brush profiles exhibit similar trends for the BNRs and MBNRs where the short grafted chain forces the longer grafted chain away from the AuNR surface and promotes wetting by the matrix chains. The hSCFT calculations demonstrated qualitative trends consistent with the aggregation observed for AuNRs in PMMA matrices. Therefore, we have demonstrated that MBNR dispersion in polymer matrices is enhanced compared to the HNR and BNR cases, which extends the dispersion window for new combinations of nanorods and polymers.

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