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### ACCEPTED MANUSCRIPT

# Mechanochemical mechanism of integrin clustering modulated by nanoscale ligand spacing and rigidity of extracellular substrates

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#### **Abstract**

Experimental findings indicate that cell function and behavior such as cell growth, division, migration and differentiation, are subtly regulated via integrin-dependent cell adhesion. Cell adhesion is influenced by nanoscale ligand spacing and rigidity of extracellular substrates, as cell adhesion drops greatly when the ligand spacing is larger than ~60nm, and cell adhesion is stronger on stiff than soft substrates. However, how nanoscale ligand spacing and substrate stiffness jointly affect integrin clustering and hence nascent cell adhesion remains to be elucidated. To quantitatively investigate the phenomena and the underlying mechanochemical mechanism of integrin clustering modulated by ligand spacing and substrate stiffness, we introduced Monte Carlo simulations varying the values of

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