

## 第 10 回量子生命科学セミナー

(4 研究科合同セミナー)

日時: 2004 年 3 月 8 日(月) 13:30 ~ 15:00

場所: 理学部 B501 室

講演題目: “**Stability of Tubulenes**”

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### **Abstract**

Tubulenes are defined as capped nanotubes built up from two generalized hemifullerene caps and a distancing nanotube portion tessellated by hexagons. Spectral regularities appearing in families of tubulenes are summarized in rules for their  $\pi$ -electronic structure, in the Hückel model.

Some new rules of thumb for their  $\pi$ -electronic stability are proposed. Strain energy is calculated in the POAV1 theory terms, for a-tubulenes, peanut z-tubulenes and peanut [5, 6, 7] tubulenes. Semiempirical calculations support the Hückel spectral data.