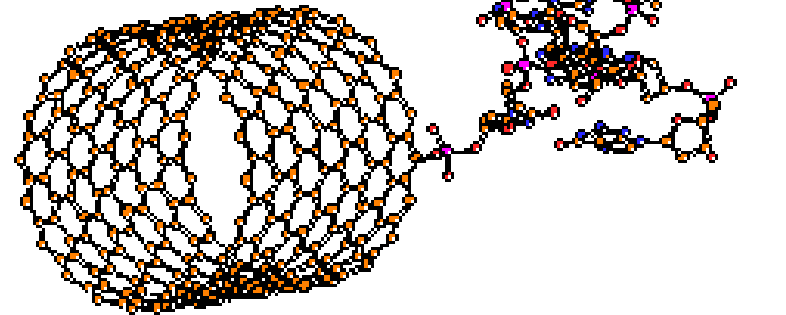
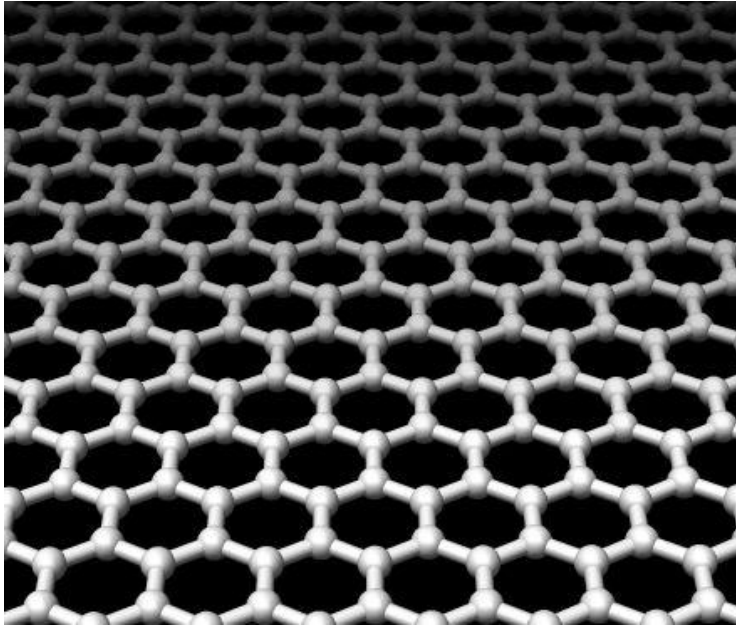
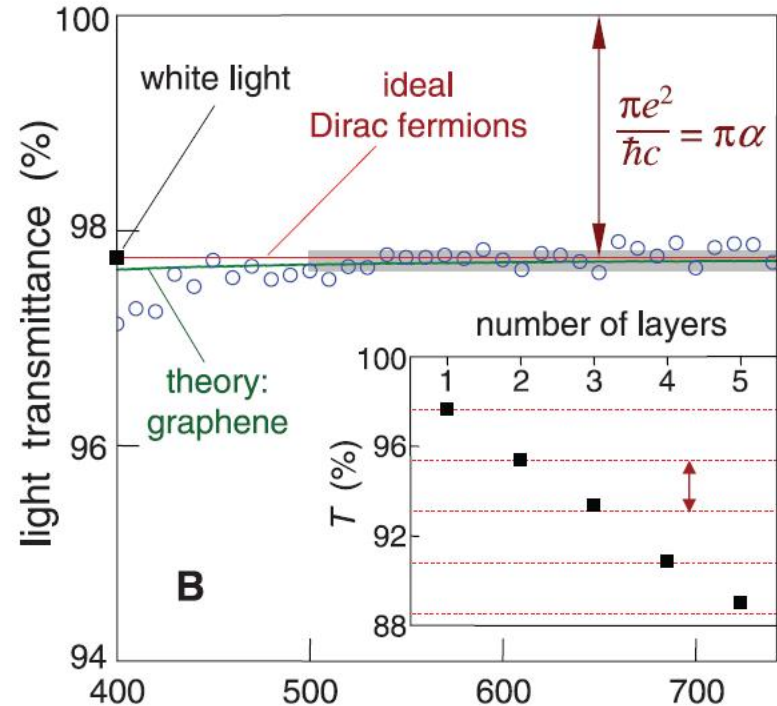
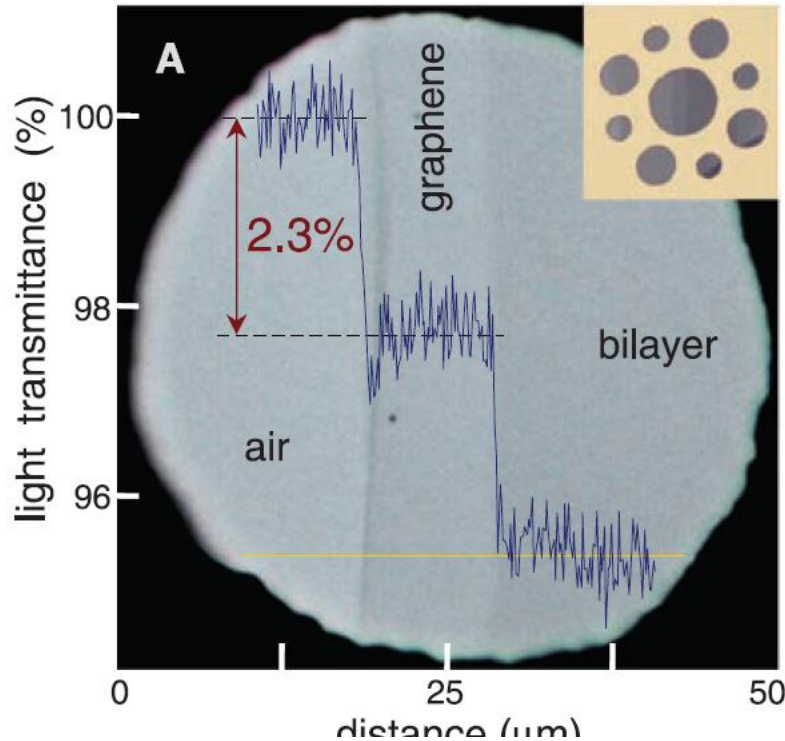


Lectures 15: Graphene optics; Nano-biotechnology



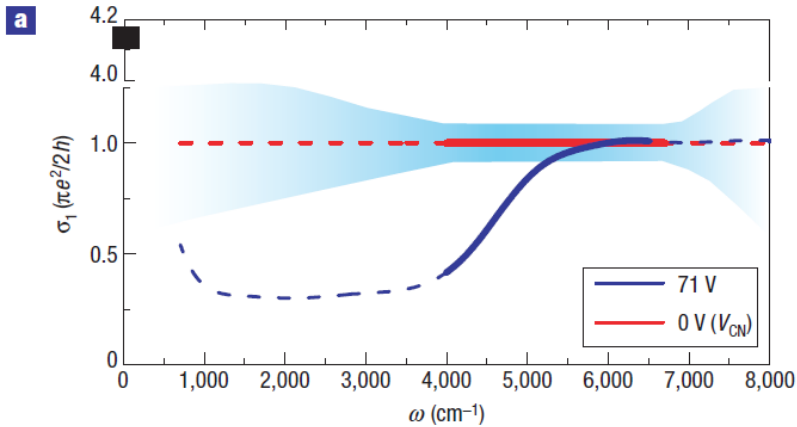
Graphene optical properties



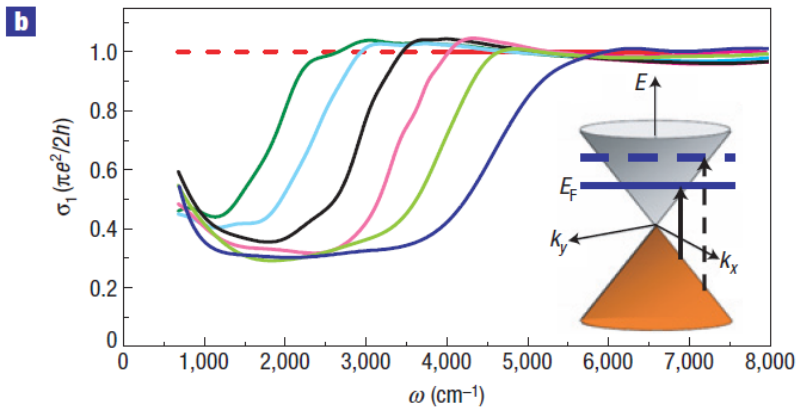
$$T_{\text{opt}} = \left(1 + \frac{\pi\alpha}{2}\right)^{-2} \approx 1 - \pi\alpha \approx 0.977$$

Nair, R. R., P. Blake, et al. (2008). "Fine Structure Constant Defines Visual Transparency of Graphene." *Science* **320**(5881): 1308.

Spectrum of absorption



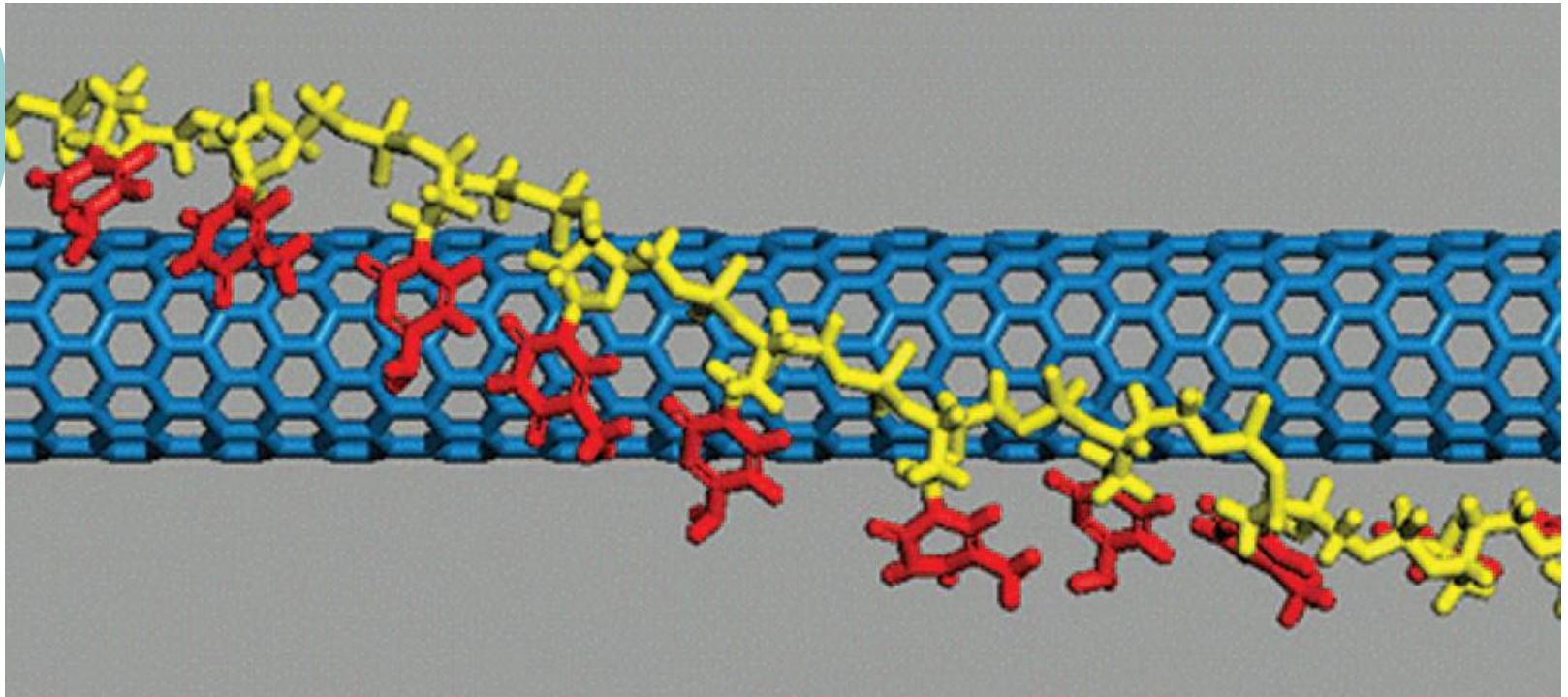
$$\text{Re } \sigma_{xx}(\Omega) = \frac{e^2}{h} |\mu| \frac{4\Gamma}{\Omega^2 + 4\Gamma^2} + \frac{\pi e^2}{2h} \theta(\Omega - 2|\mu|).$$



Li, Z., E. Henriksen, et al. (2008). "Dirac charge dynamics in graphene by infrared spectroscopy." *Nature Physics* **4**(7): 532-535.

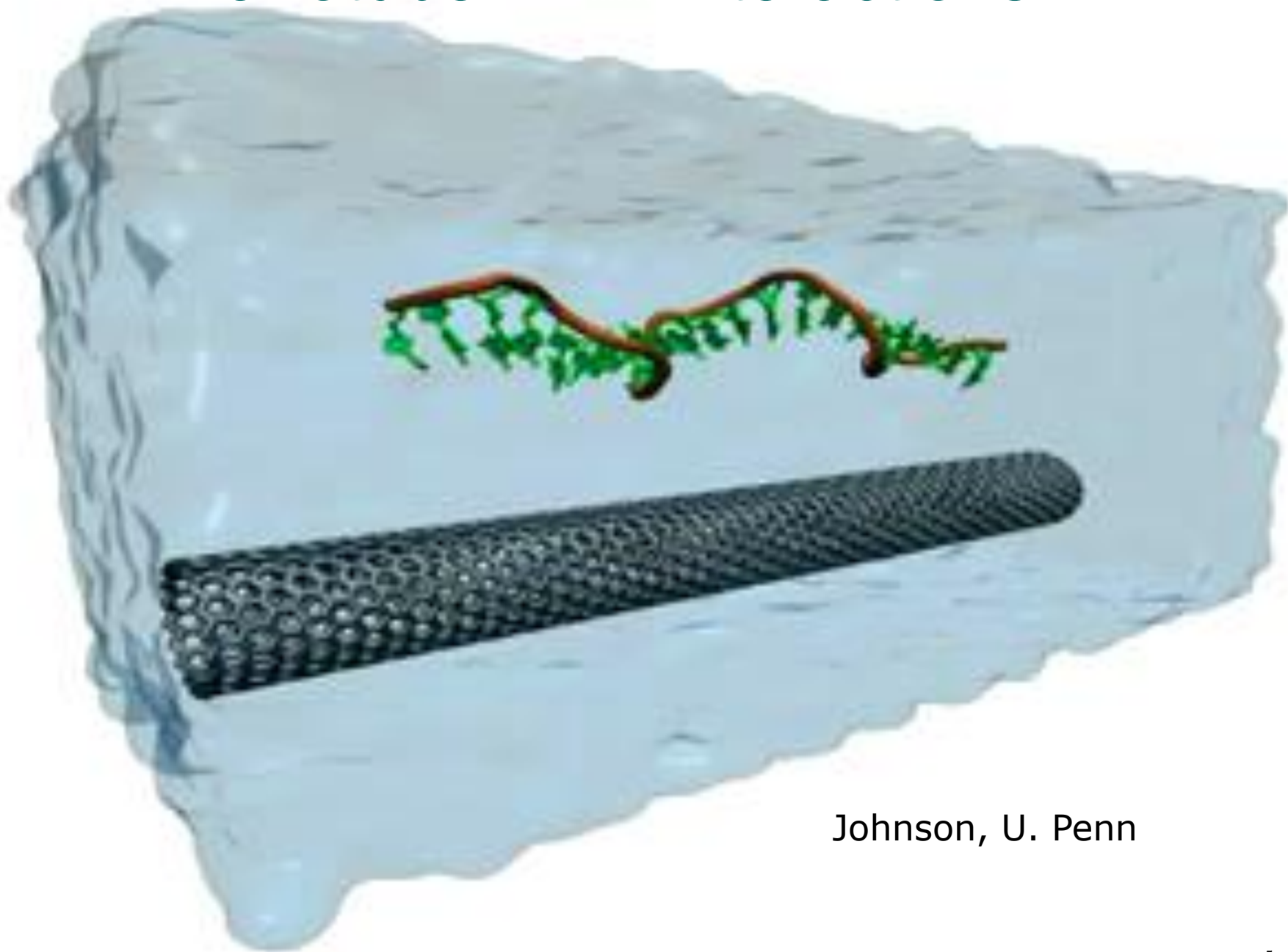
Gusynin, V., S. Sharapov, et al. (2009). "On the universal ac optical background in graphene." *New Journal of Physics* **11**: 095013.

Nanotube-DNA interactions



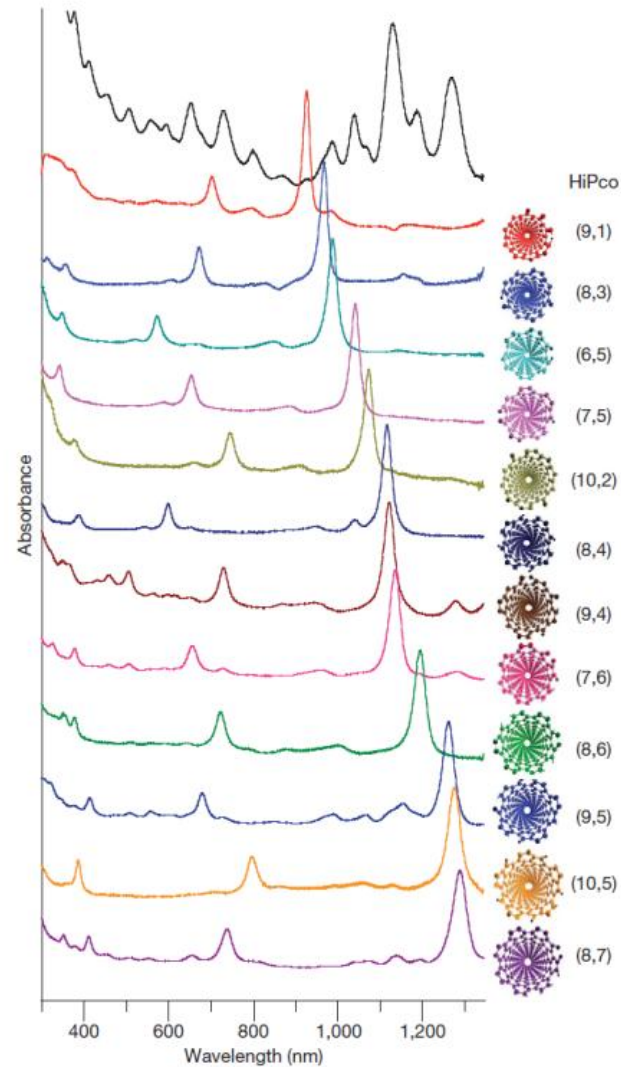
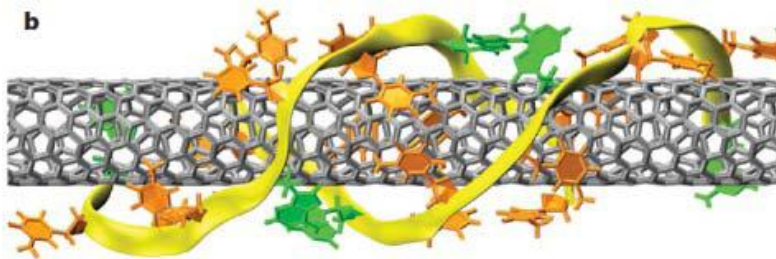
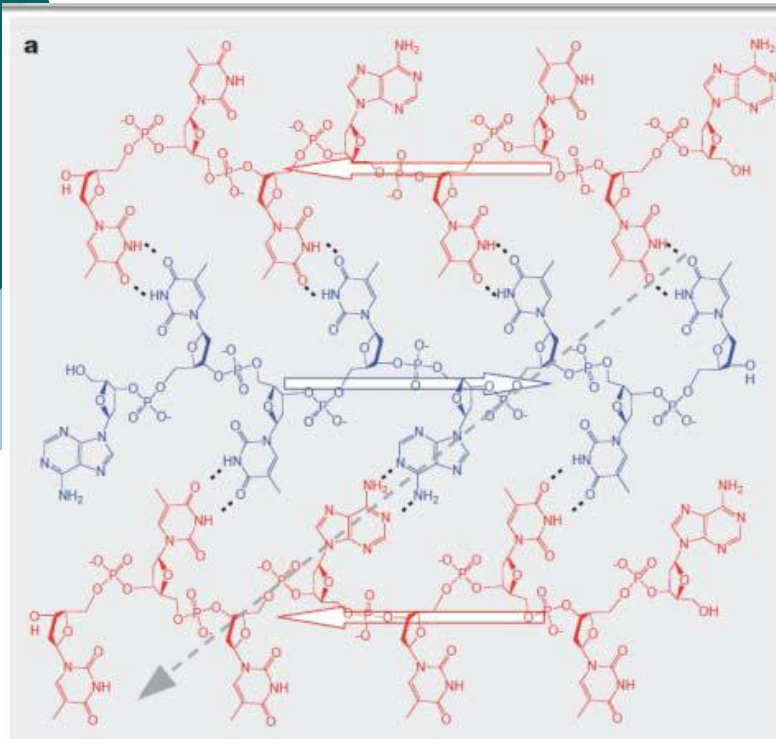
X. Tu and M. Zheng, "A DNA-Based Approach to the Carbon Nanotube Sorting Problem", *Nano Research*, **1**, 185-194, **(2008)**.

Nanotube-DNA interactions



Johnson, U. Penn

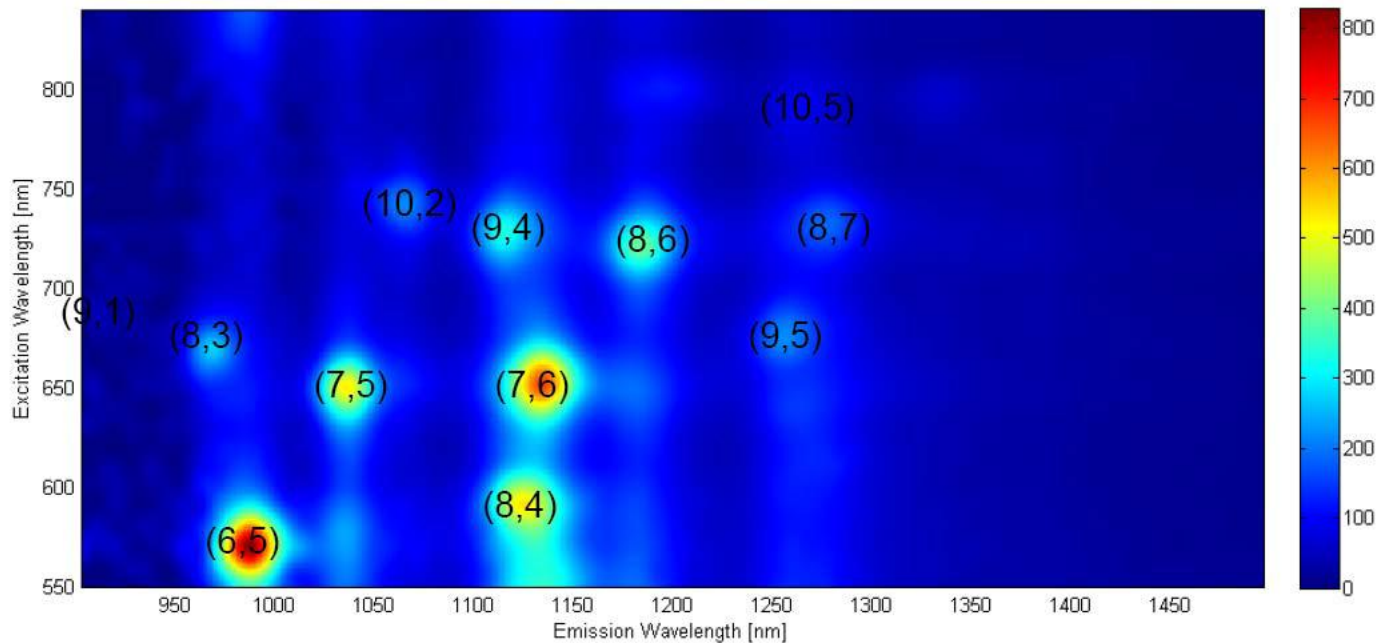
Sequence specificity



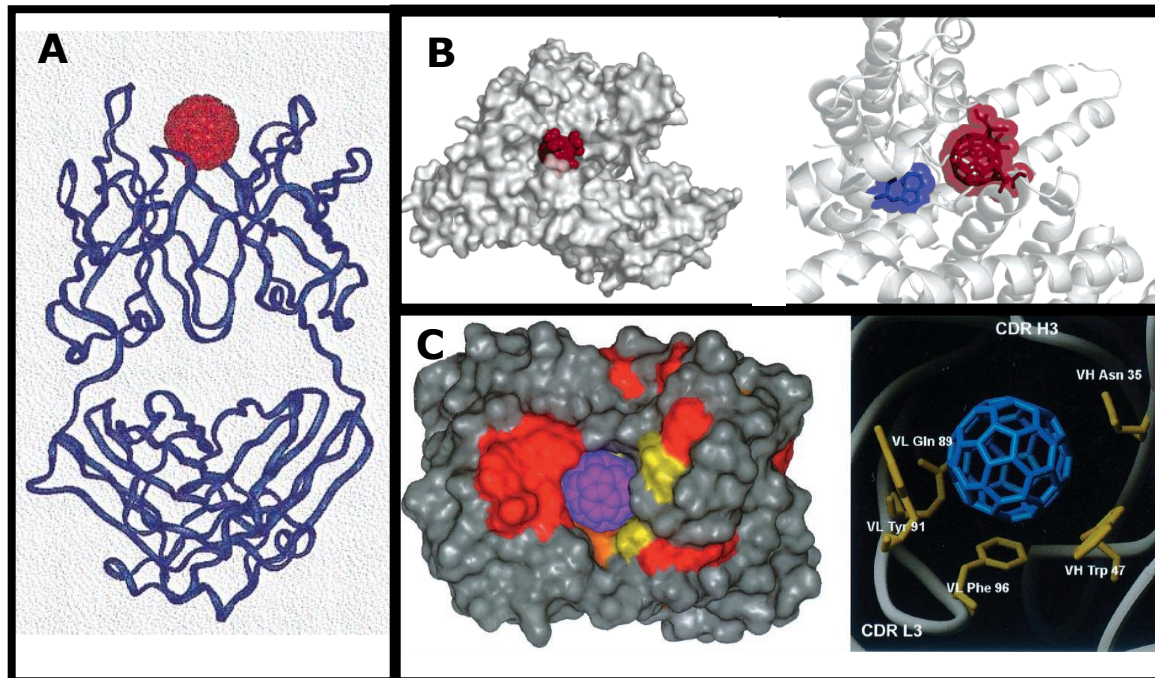
- | | |
|--------|---|
| HiPco | (9,1) (TCC)10,
(TGA)10, (CCA)10 |
| (9,1) | (8,3) (TTA)4TT,
(TTA)3TTGTT,
(TTA)5TT |
| (8,3) | (6,5) (TAT)4, (CGT)3C |
| (6,5) | (7,5) (ATT)4,
(ATT)4AT |
| (7,5) | (10,2) (TATT)2TAT |
| (10,2) | (8,4) (ATTT)3 |
| (8,4) | (9,4) (GTC)2GT,
(CCG)4 |
| (9,4) | (7,6) (GTT)3G,
(TGT)4T |
| (7,6) | (8,6) (GT)6, (TATT)3T,
(TCG)10, (GTC)3,
(TCG)2TC,
(TCG)4TC, (GTC)2 |
| (8,6) | (9,5) (TGTT)2TGT |
| (9,5) | (10,5) (TTTA)3T |
| (10,5) | (8,7) (CCG)2CC |
| (8,7) | |

X. Tu, S. Manohar, A. Jagota and M. Zheng, "DNA Sequence Motifs for Structure-Specific Recognition and Separation of Carbon Nanotubes", *Nature*, 460, 250-253, (2009).

Flourescence nanotube species determination



C60 – antibody interactions



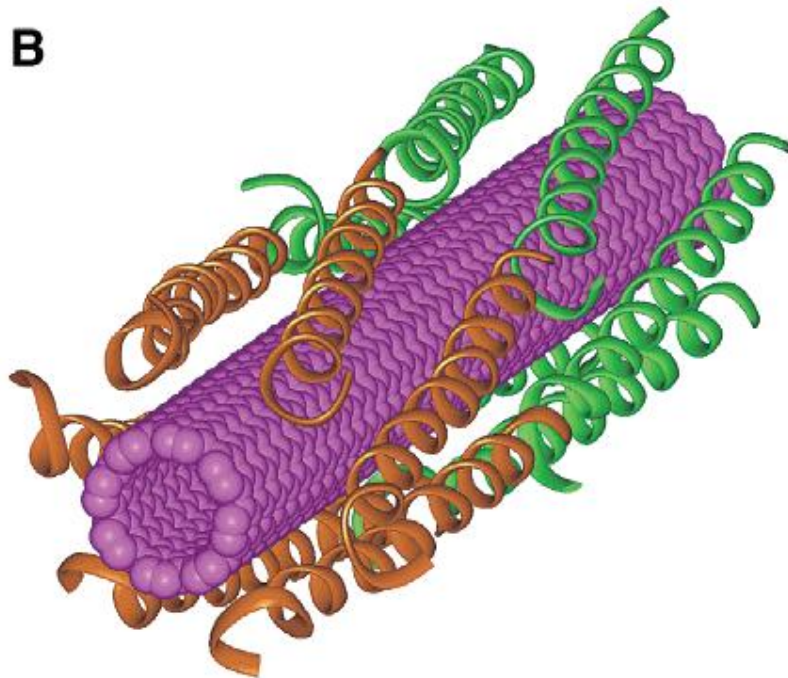
B. C. Braden, F. A. Goldbaum, B. X. Chen, A. N. Kirschner, S. R. Wilson and B. F. Erlanger, "X-Ray Crystal Structure of an Anti-Buckminsterfullerene Antibody Fab Fragment: Biomolecular Recognition of C-60", *Proceedings of the National Academy of Sciences of the United States of America*, **97**, 12193- 12197, (2000).

[18.] B. X. Chen, S. R. Wilson, M. Das, D. J. Coughlin and B. F. Erlanger, "Antigenicity of Fullerenes: Antibodies Specific for Fullerenes and Their Characteristics", *Proceedings of the National Academy of Sciences of the United States of America*, **95**, 10809-10813, (1998).

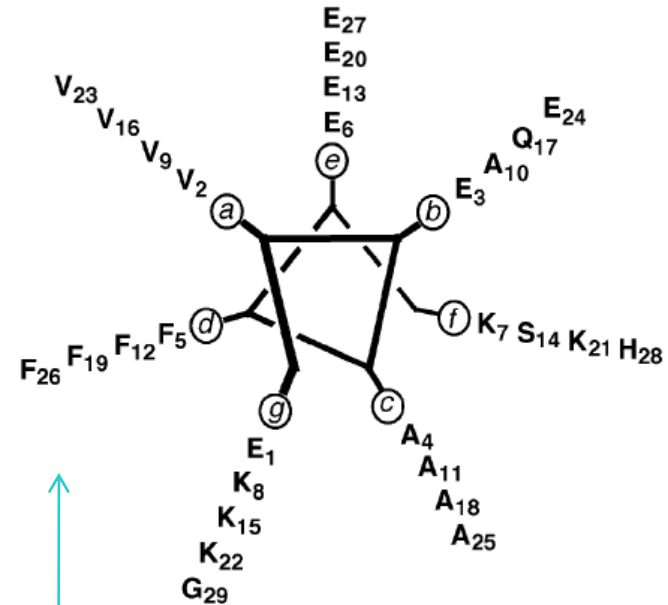
[19.] B. F. Erlanger, B. X. Chen, M. Zhu and L. Brus, "Binding of an Anti-Fullerene IgG Monoclonal Antibody to Single Wall Carbon Nanotubes", *Nano Letters*, **1, b** (2001).

[20.] B. Belgorodsky, L. Fadeev, V. Ittah, H. Benyamini, S. Zelner, D. Huppert, A. B. Kotlyar and M. Gozin, "Formation and Characterization of Stable Human Serum Albumin-Tris-Malonic Acid [C-60]Fullerene Complex", *Bioconjugate Chemistry*, **16**, 1058-1062, (2005).

Nanotube-peptide interactions



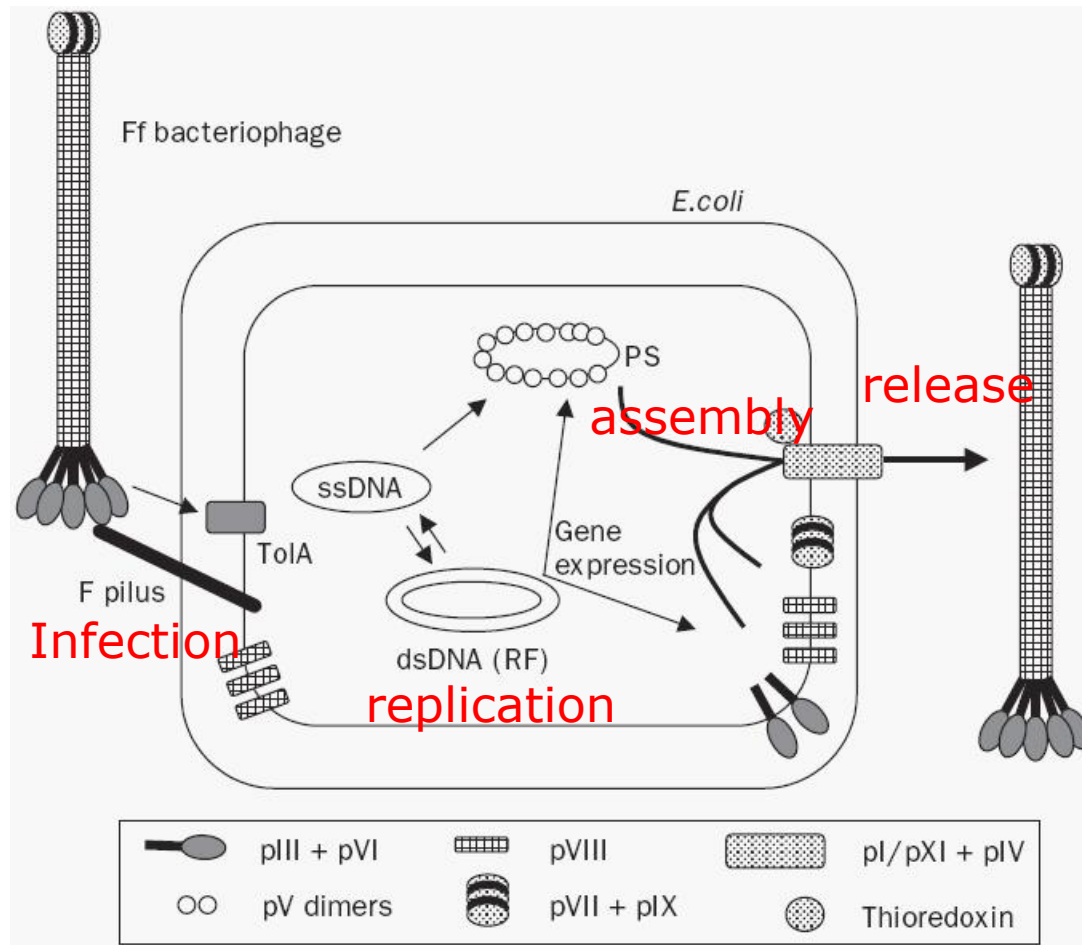
Helical wheel projection



G. R. Dieckmann, A. B. Dalton, P. A. Johnson, J. Razal, J. Chen, G. M. Giordano, E. Munoz, I. H. Musselman, R. H. Baughman and R. K. Draper, "Controlled Assembly of Carbon Nanotubes by Designed Amphiphilic Peptide Helices", *Journal of the American Chemical Society*, **125**, 1770-1777, (2003).

hydrophobic

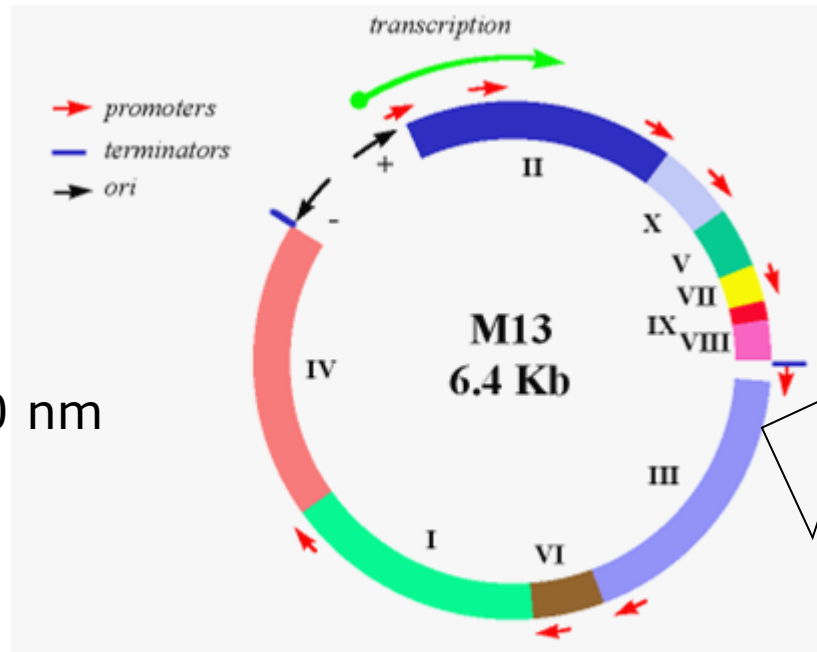
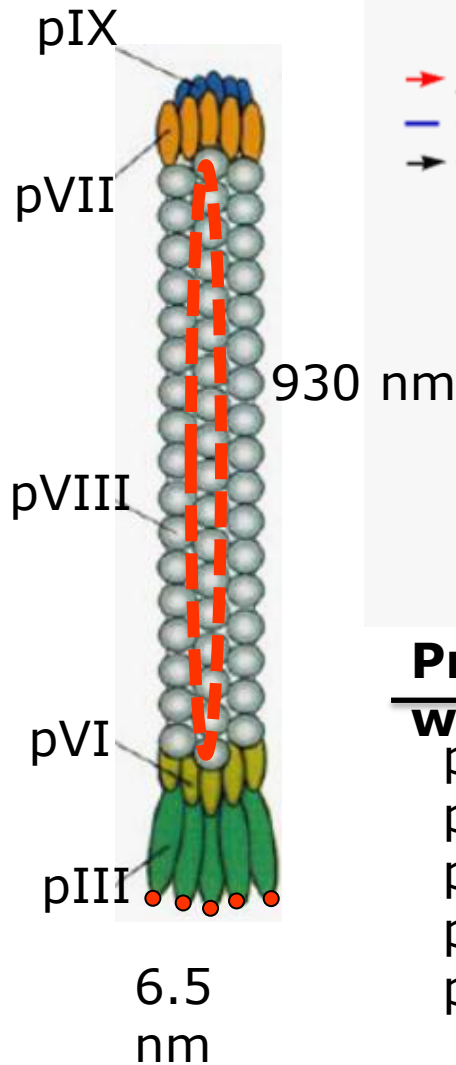
Phage virus life cycle



After 10 minutes of infection, the 1st generation of phage
 Rate: 1000 / cell / hour

M. Russel, Phage display, Oxford Press, 2004

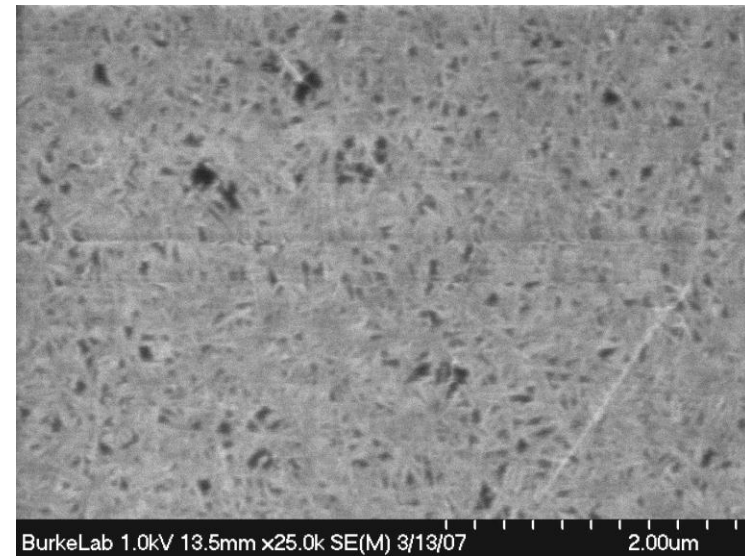
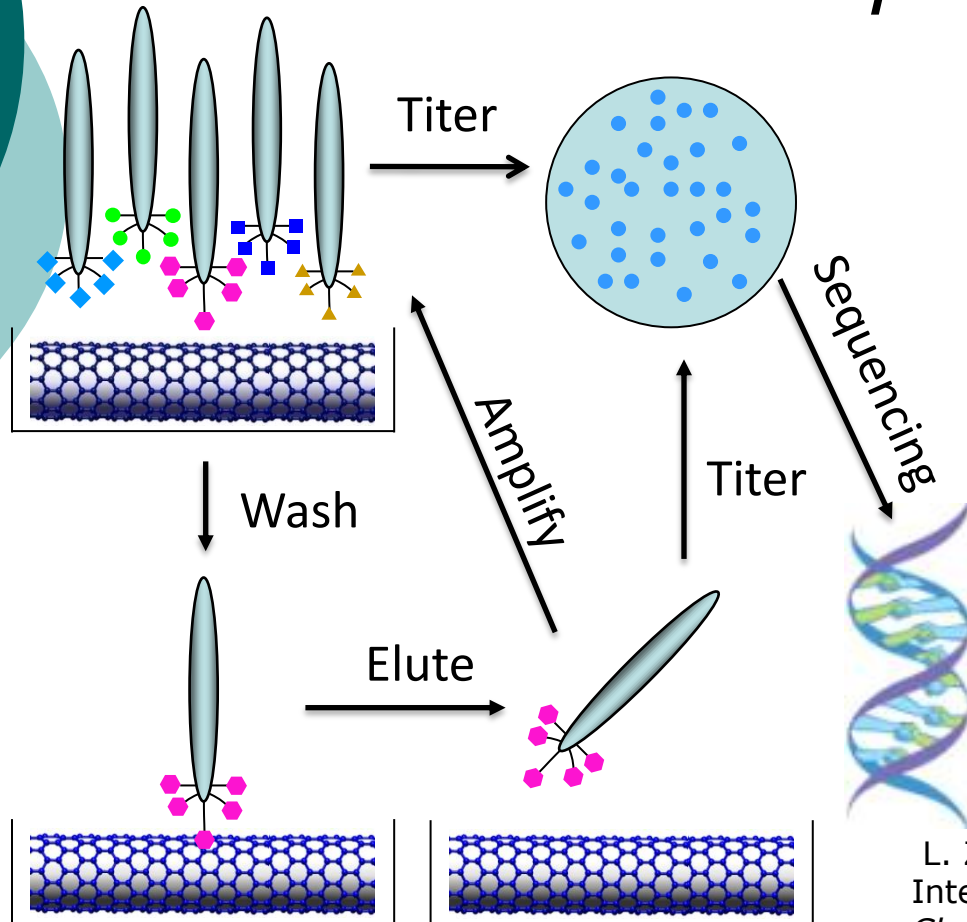
Structure of bacteriophage M13



Protein	AA numbers	Mol.	Copies
pIII	405	42,500	5
pVI	112	12,300	5
pVII	33	3,600	5
pVIII	50	5,200	2700
pIX	32	3,600	5

Phage display

Schematic procedure



L. Zheng, D. Jain and P. Burke, "Nanotube Peptide Interactions on a Silicon Chip", *The Journal of Physical Chemistry C*, **113**, 3978-3985, (2009).

Binding sequences

TABLE 1: Sequences of Peptides Bound to Single-Walled Carbon Nanotubes

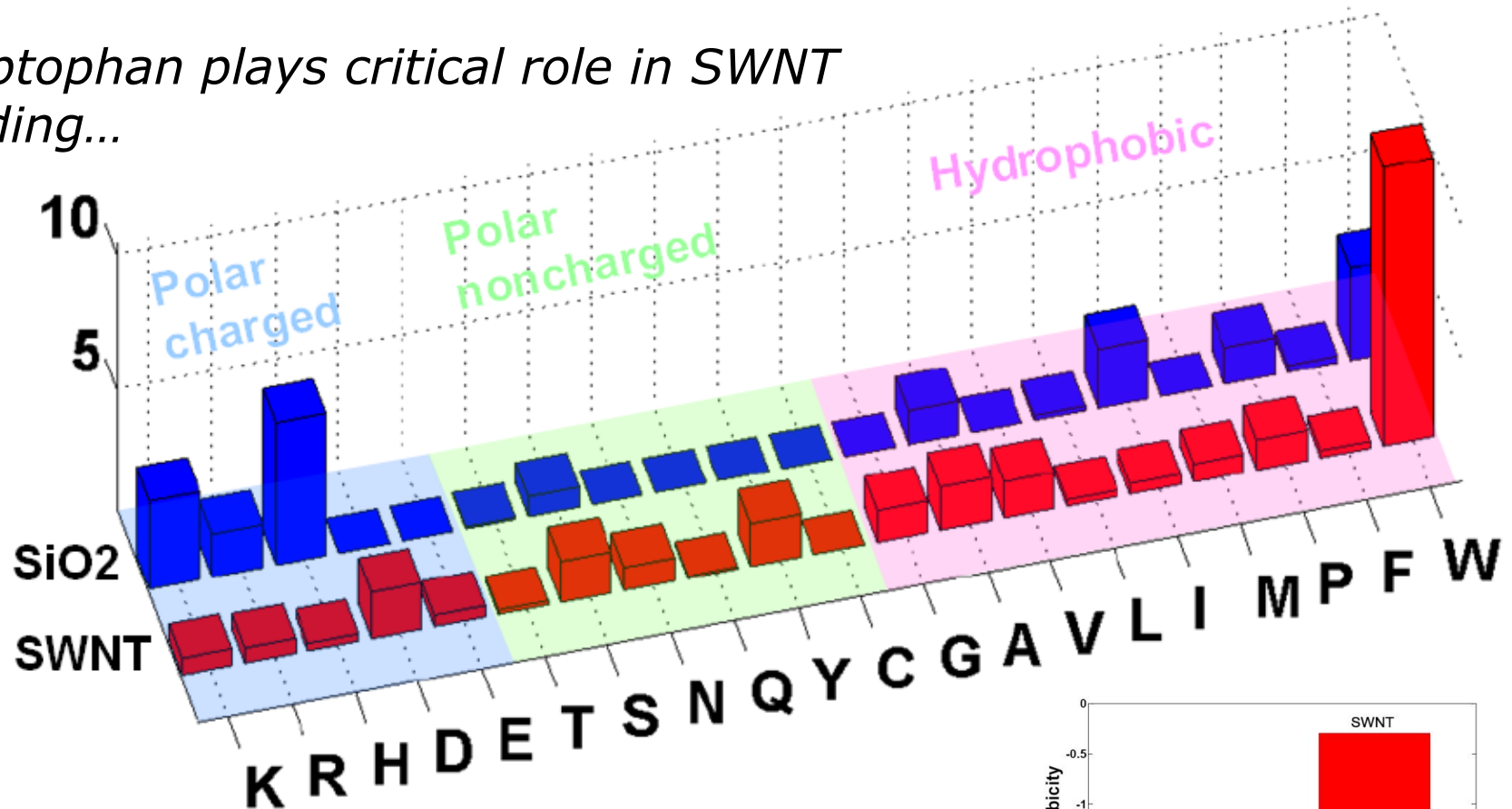
no.	amino acids												occurrence
P1	D	D	W	S	H	W	W	R	A	W	N	G	3
P2	Y	T	S	P	W	W	L	A	W	Y	D	P	2
P3	A	W	W	E	A	F	I	P	N	S	I	T	1
P4	W	F	P	I	A	W	P	E	S	W	Y	H	1
P5	G	W	D	W	A	Q	D	W	N	W	W	T	1
P6	N	D	N	P	W	L	M	W	L	K	N	W	1
P7	Y	E	Y	P	W	A	N	W	W	L	S	P	1
P8	S	S	A	W	W	S	Y	W	P	P	V	A	6

Side chain properties

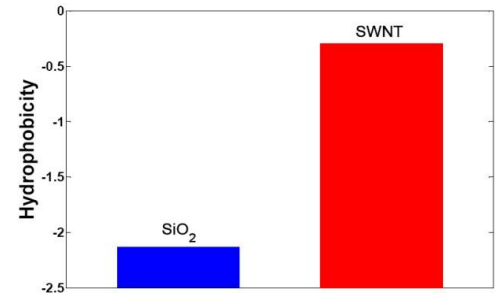
Amino Acid	Short	Abbrev.	Side chain	Hydro-phobic	pKa	Polar	pH	Small	Tiny	Aromatic or Aliphatic	van der Waals volume
Alanine	A	Ala	-CH ₃	X	-	-	-	X	X	-	67
Cysteine	C	Cys	-CH ₂ SH	X	8.18	-	acidic	X	-	-	86
Aspartic acid	D	Asp	-CH ₂ COOH	-	3.90	X	acidic	X	-	-	91
Glutamic acid	E	Glu	-CH ₂ CH ₂ COOH	-	4.07	X	acidic	-	-	-	109
Phenylalanine	F	Phe	-CH ₂ C ₆ H ₅	X	-	-	-	-	-	Aromatic	135
Glycine	G	Gly	-H	X	-	-	-	X	X	-	48
Histidine	H	His	-CH ₂ -C ₃ H ₃ N ₂	-	6.04	X	weak basic	-	-	Aromatic	118
Isoleucine	I	Ile	-CH(CH ₃)CH ₂ CH ₃	X	-	-	-	-	-	Aliphatic	124
Lysine	K	Lys	-(CH ₂) ₄ NH ₂	-	10.54	X	basic	-	-	-	135
Leucine	L	Leu	-CH ₂ CH(CH ₃) ₂	X	-	-	-	-	-	Aliphatic	124
Methionine	M	Met	-CH ₂ CH ₂ SCH ₃	X	-	-	-	-	-	-	124
Asparagine	N	Asn	-CH ₂ CONH ₂	-	-	X	-	X	-	-	96
Pyrrolysine	O	Pyl									
Proline	P	Pro	-CH ₂ CH ₂ CH ₂ -	X	-	-	-	X	-	-	90
Glutamine	Q	Gln	-CH ₂ CH ₂ CONH ₂	-	-	X	-	-	-	-	114
Arginine	R	Arg	-(CH ₂) ₃ NH-C(NH)NH ₂	-	12.48	X	strongly basic	-	-	-	148
Serine	S	Ser	-CH ₂ OH	-	-	X	-	X	X	-	73
Threonine	T	Thr	-CH(OH)CH ₃	-	-	X	weak acidic	X	-	-	93
Selenocysteine	U	Sec	-CH ₂ SeH	X	5.73	-	-	X	-	-	
Valine	V	Val	-CH(CH ₃) ₂	X	-	-	-	X	-	Aliphatic	105
Tryptophan	W	Trp	-CH ₂ C ₈ H ₆ N	X	-	-	-	-	-	Aromatic	163
Tyrosine	Y	Tyr	-CH ₂ -C ₆ H ₄ OH	-	10.46	X	-	-	-	Aromatic	141

Relative occurrence of amino acids

Tryptophan plays critical role in SWNT binding...

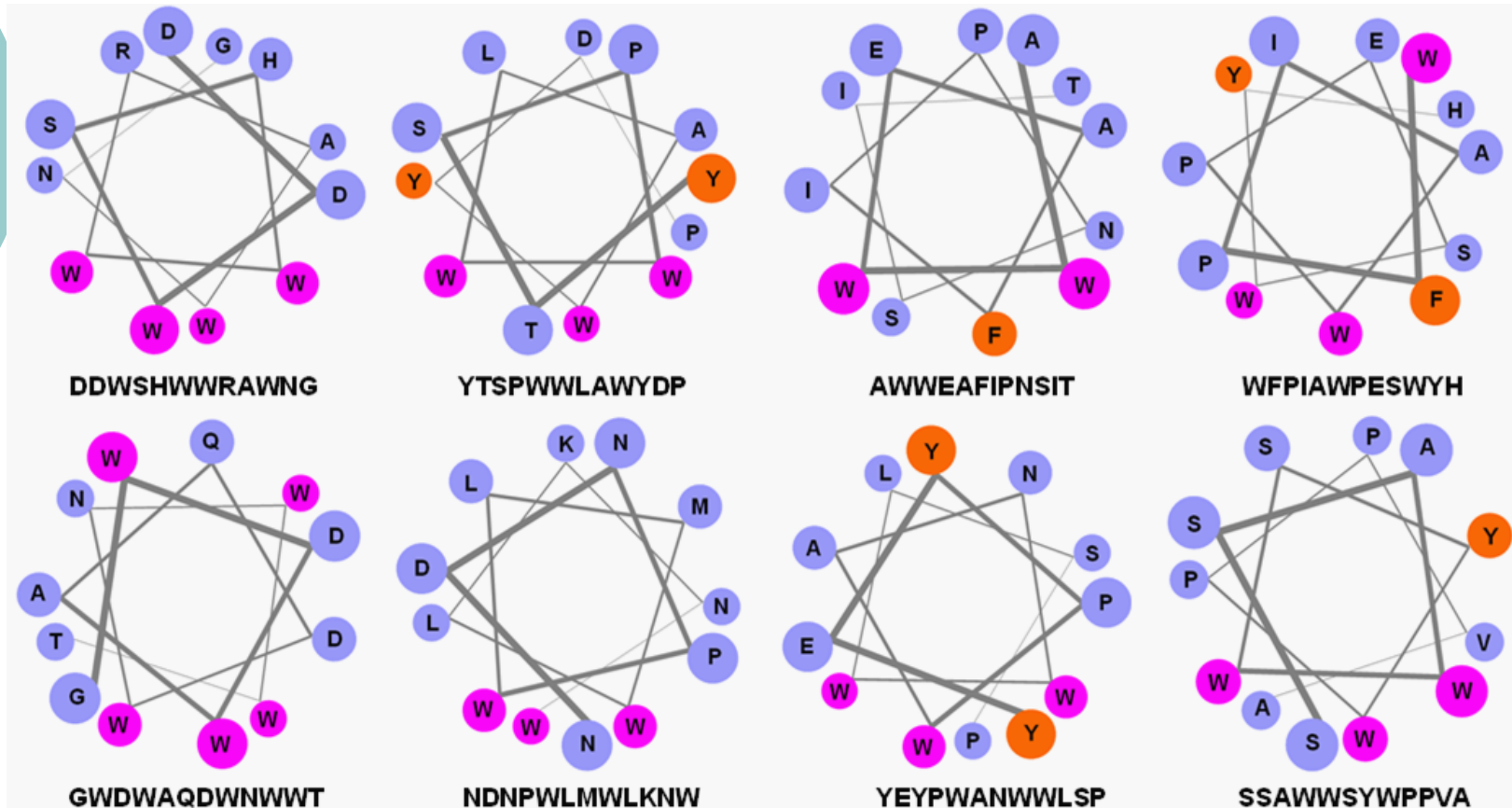


L. Zheng, D. Jain and P. Burke, "Nanotube Peptide Interactions on a Silicon Chip", *The Journal of Physical Chemistry C*, **113**, 3978-3985, (2009).



Helical wheel

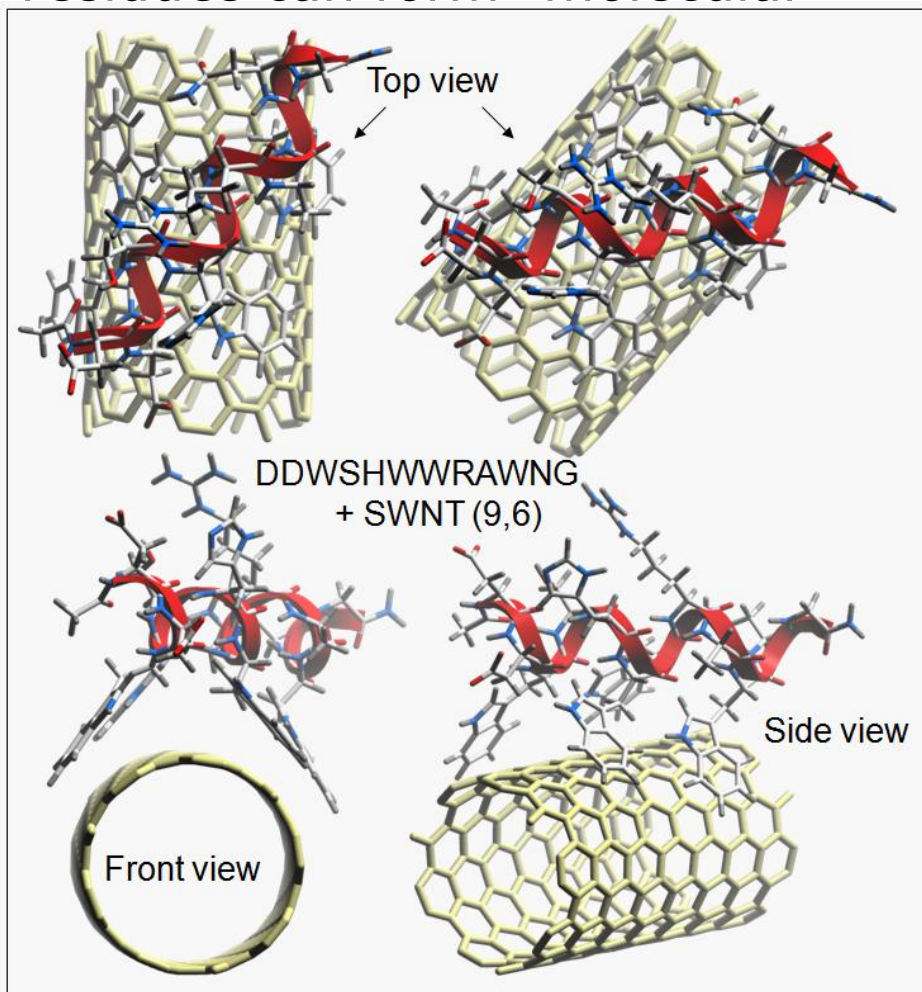
Tryptophan residues aligned on one side of α -helix



L. Zheng, D. Jain and P. Burke, "Nanotube Peptide Interactions on a Silicon Chip", *The Journal of Physical Chemistry C*, **113**, 3978-3985, (2009).

Nanotube-peptide docking

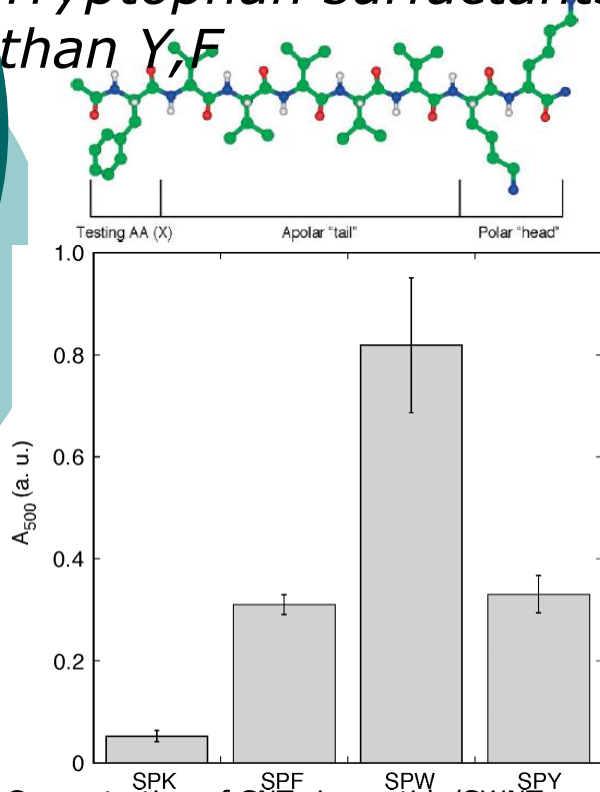
Tryptophan residues can form "molecular tweezers"



L. Zheng, D. Jain and P. Burke, "Nanotube Peptide Interactions on a Silicon Chip", *The Journal of Physical Chemistry C*, **113**, 3978-3985, (2009).

Tryptophan-SWNT binding

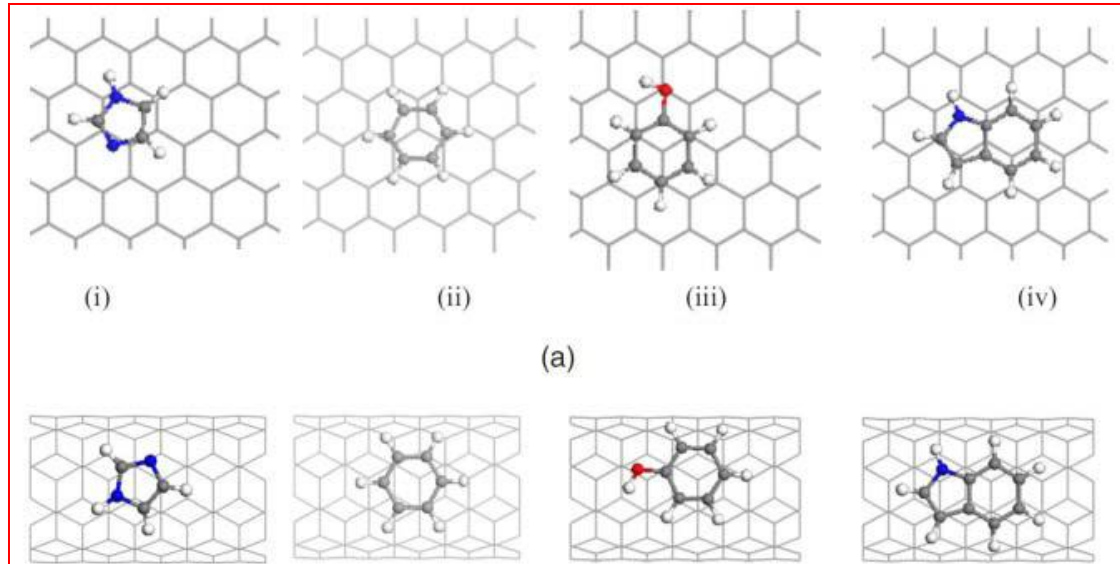
Tryptophan surfactants dissolves SWNTs more effectively than Y,F



Concentration of CNTs in peptide/SWNT dispersions after 16, 000 g-centrifugation step. The absorbance at

500 nm is used as a measure of CNT

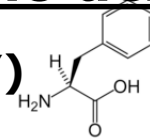
Concentration. R. H. Baughman, A. B. Dalton and G. D. Stucky, "Ranking the Affinity of Aromatic Residues for Carbon Nanotubes by Using Designed Peptide Surfactants", *Journal of Peptide Science*, **14**, 139-151, (2008).



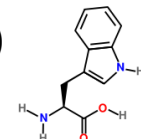
C. Rajesh, C. Majumder, H. Mizuseki and Y. Kawazoe, "A Theoretical Study on the Interaction of Aromatic Amino Acids with Graphene and Single Walled Carbon Nanotube", *The Journal of Chemical Physics*, **130**, 124911, (2009).

Aromatic amino acids

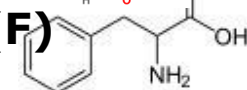
Tyrosine (Y)



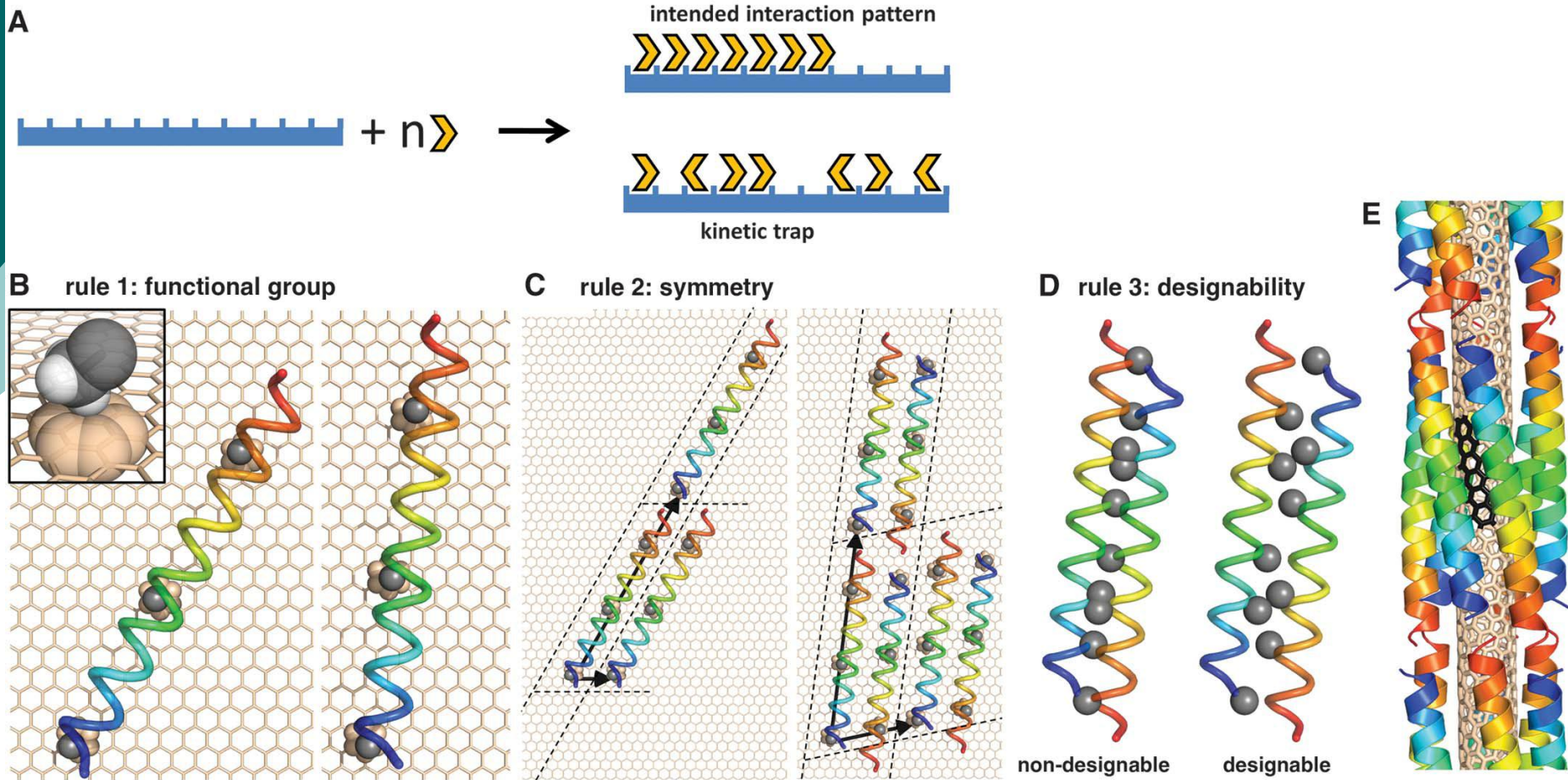
Tryptophan (W)



Phenylalanine (F)



Protein-Nanotube sorting

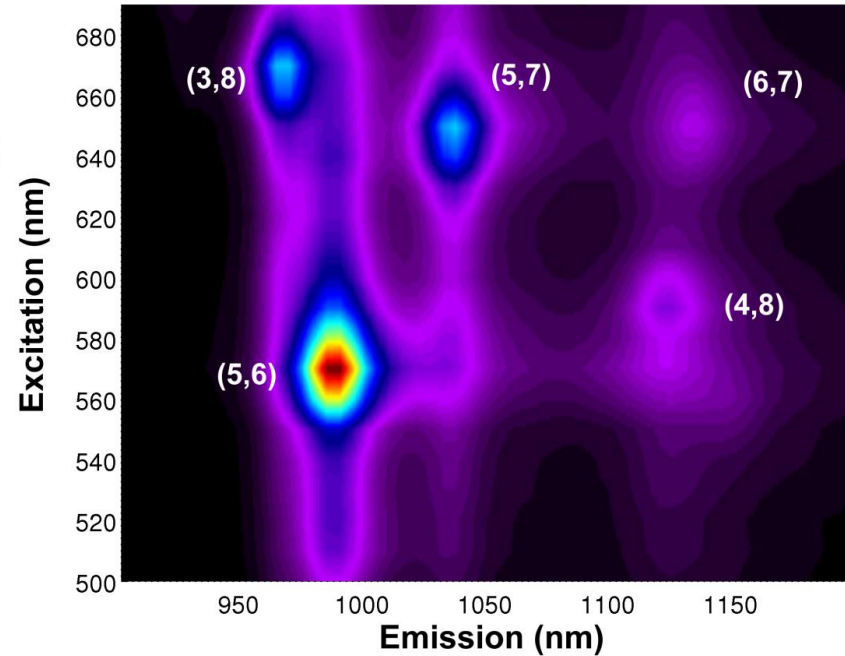
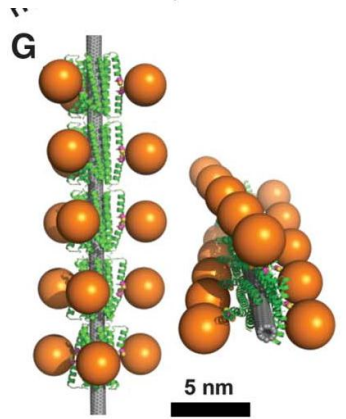
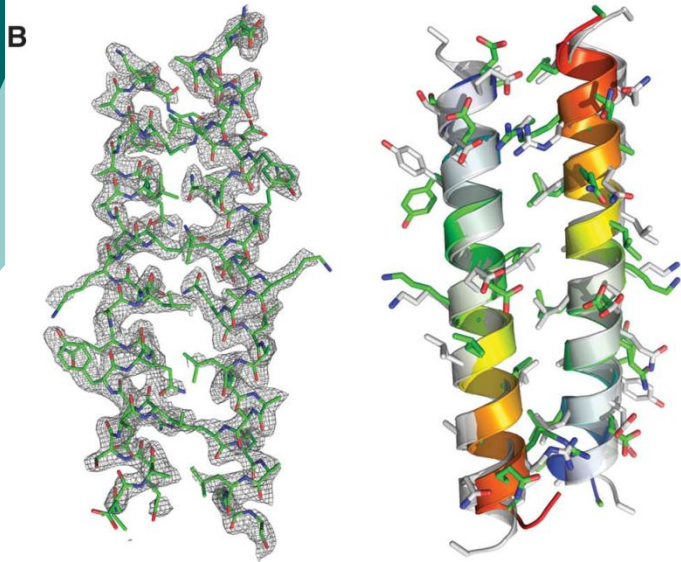
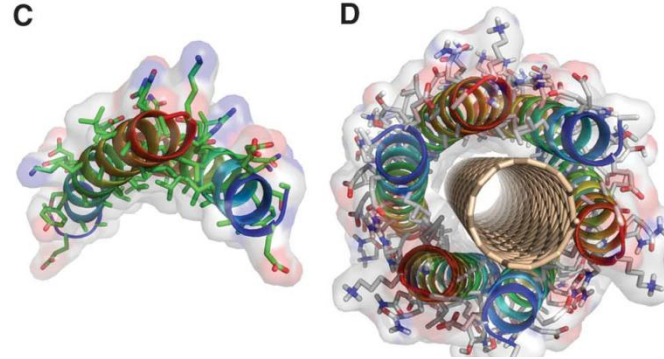


Grigoryan, G., Y. H. Kim, et al. (2011). "Computational Design of Virus-Like Protein Assemblies on Carbon Nanotube Surfaces." *Science* **332**(6033): 1071-1076.

Protein-Nanotube sorting

A heptad register

HexCoil-Gly	fgabcdefgabcdefgabcdefgabcdefg
HexCoil-Ala	AEGESALEYGGQALEKGLALQAGRQALKA
cHexCoil-Gly	AEAESALEYQQALEKAQLALQAAARQALKA
cHexCoil-Ala	AELESGAEYLLQQAQAEKLLQGAQALRQGAKA
Native DSD	SLAALKSELQALKKEGFSPEELAALESLELQALEKKLAALKSKLQALKG
DSD-Gly	SLAALKSELQALKKEGFSPEGLAALESGLQALEKGLAALKSGLQALKG
DSD-Ala	SLAALKSELQALKKEGFSPEALAALESALQALEKALAALKSALQALKG
DSD-His	SLAALKSELQALKKEGFSPEGLAALESHLQALEKHLAALKSGLQALKG



Grigoryan, G., Y. H. Kim, et al. (2011). "Computational Design of Virus-Like Protein Assemblies on Carbon Nanotube Surfaces." *Science* **332**(6033): 1071-1076.