

# Publikationsliste: Stand 7.7.2010

Im Folgenden werden Referenzen aus der Publikationsliste meinen Arbeitsschwerpunkten zugeordnet:

## Methodenentwicklung

- Entwicklung und Erweiterung der approximativen Dichtefunktionalmethode SCC-DFTB: [3, 97, 98, 99, 7, 8, 15, 18, 22, 25, 103, 32, 62, 67, 70, 71, 73, 82].
- Entwicklung von kombinierten quantenmechanischen/klassischen Methoden (QM/MM): [10, 12, 30, 36, 68, 69, 105].
- Multi-Skalen-Methoden: Kombination von QM mit MM und Kontinuumsbeschreibungen [59, 60, 106]
- Quantenmechanische Beschreibung optisch angeregter Zustände und Photobiophysik: [16, 21, 42, 53, 63, 64, 78, 79].
- Methoden zur Beschreibung von Elektronentransport durch organische Moleküle und DNA [38, 43, 56, 75, 91, 95].

## Anwendungsgebiete

- Beschreibung von Ladungstransportprozessen in biologischen Systemen: Protonentransport [12, 23, 40, 47, 50, 51, 59, 65, 66, 81, 86, 89] und Elektronentransport in DNA [29, 76, 77, 83, 87, 88, 84, 90, 94].
- Struktur und Stabilität von Polypeptiden und Proteinen: [4, 5, 9, 17, 20, 30, 46].
- Struktur und Stabilität von DNA Basenpaaren und DNA: [15, 26, 34, 35, 37].
- Wechselwirkung von biologischen/organischen Molekülen mit Festkörperoberflächen: [11, 38, 49, 55]
- Simulation der Eigenschaften und Dynamik von Kohlenstoff-Nanoröhren und Fullerenen: [101, 102, 33, 39, 45, 104, 61].
- Festkörper, Oberflächen, Molekülkristalle: [1, 6, 13, 14, 19, 27, 28]

## Ethische und Soziale Aspekte der Biowissenschaften

- Marcus Elstner (Hrg.): Gentechnik und Ethik, Springer Verlag 1997
- T. Braun, M. Elstner (Hrg.): Gene und Gesellschaft, Deutsches Krebsforschungszentrum, Heidelberg 1999
- M. Elstner, N. Gottschalk: Rezension des Buches "Bioethik" von F. Zülke, Spektrum der Wissenschaft 2/98, S.130

## Die 10 meist zitierten Veröffentlichungen

(Stand 7.7.20010 nach ISI web of science ohne Ausschluss der eigenen Zitationen)

<b>Zitate</b>	<b>Referenz</b> (in der nachfolgenden Publikationsliste)
755	[3]
396	[48]
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**Hirsch-Index (h-index): 32**

### **Publikationen nach ausgewählten Zeitschriften:**

(in Klammern die Referenz in der nachfolgenden Publikationsliste)

- Proc. Natl. Acad. Sci. (USA) [81]
- J. Am. Chem. Soc. [26, 51, 63, 65, 86]
- Nano Letters [33, 39, 77]
- J. Mol. Bio. [48]
- Structure [47]
- Proteins [20, 30]
- Biochemistry [31]
- J. Struc. Biol. [66]
- J. Phys. Chem. [4, 12, 23, 28, 45, 53, 59, 60, 61, 67, 68, 69, 70, 71, 73, 75, 76, 78, 79, 83, 88]
- J. Chem. Phys. [15, 27, 42, 54, 80, 87]
- Phys. Rev. Lett. [1, 13, 84]
- Phys. Rev. B [3, 6, 11, 14, 16, 19, 21, 29, 38, 44, 56, 57]

## Literatur

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