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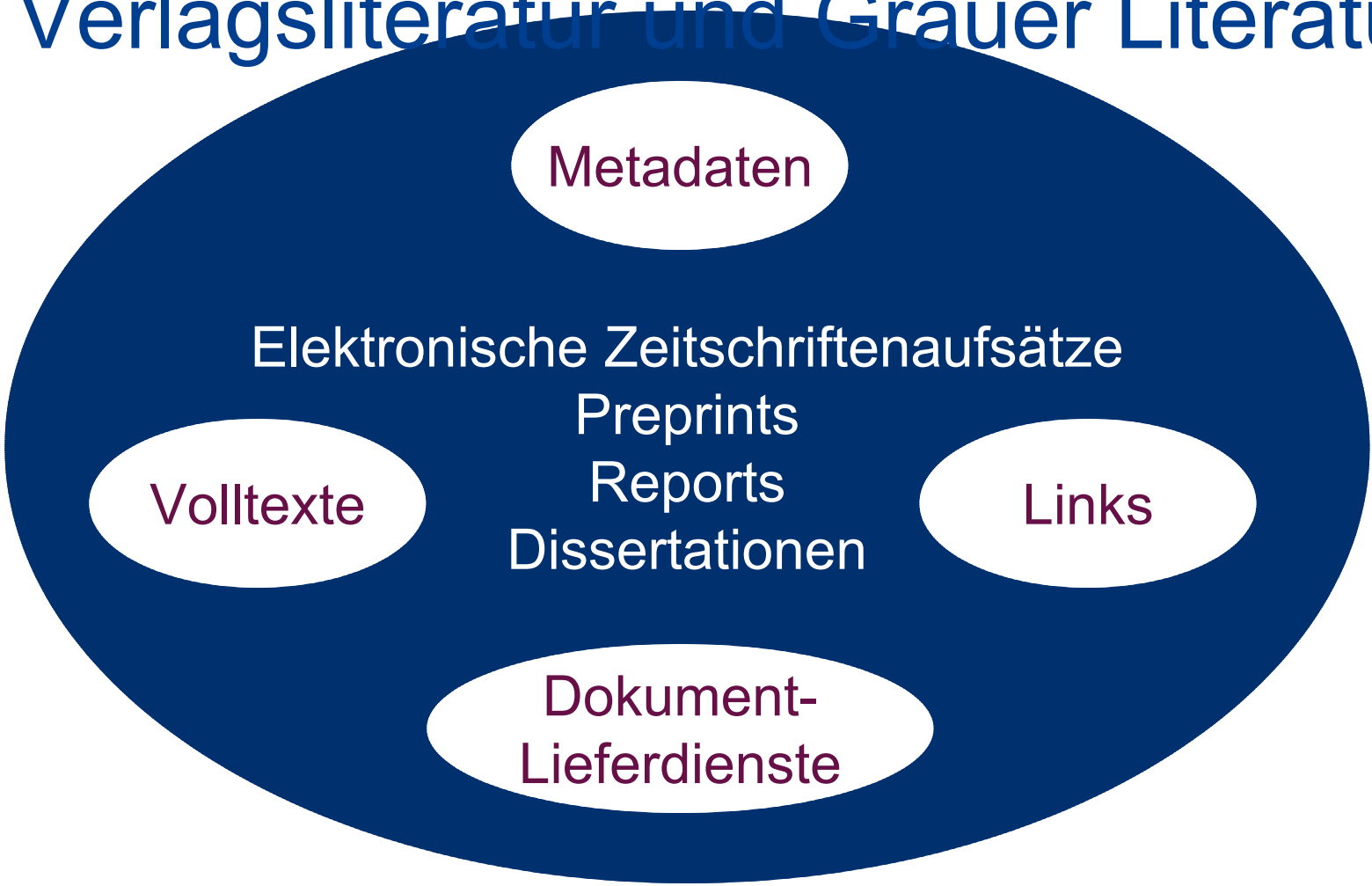

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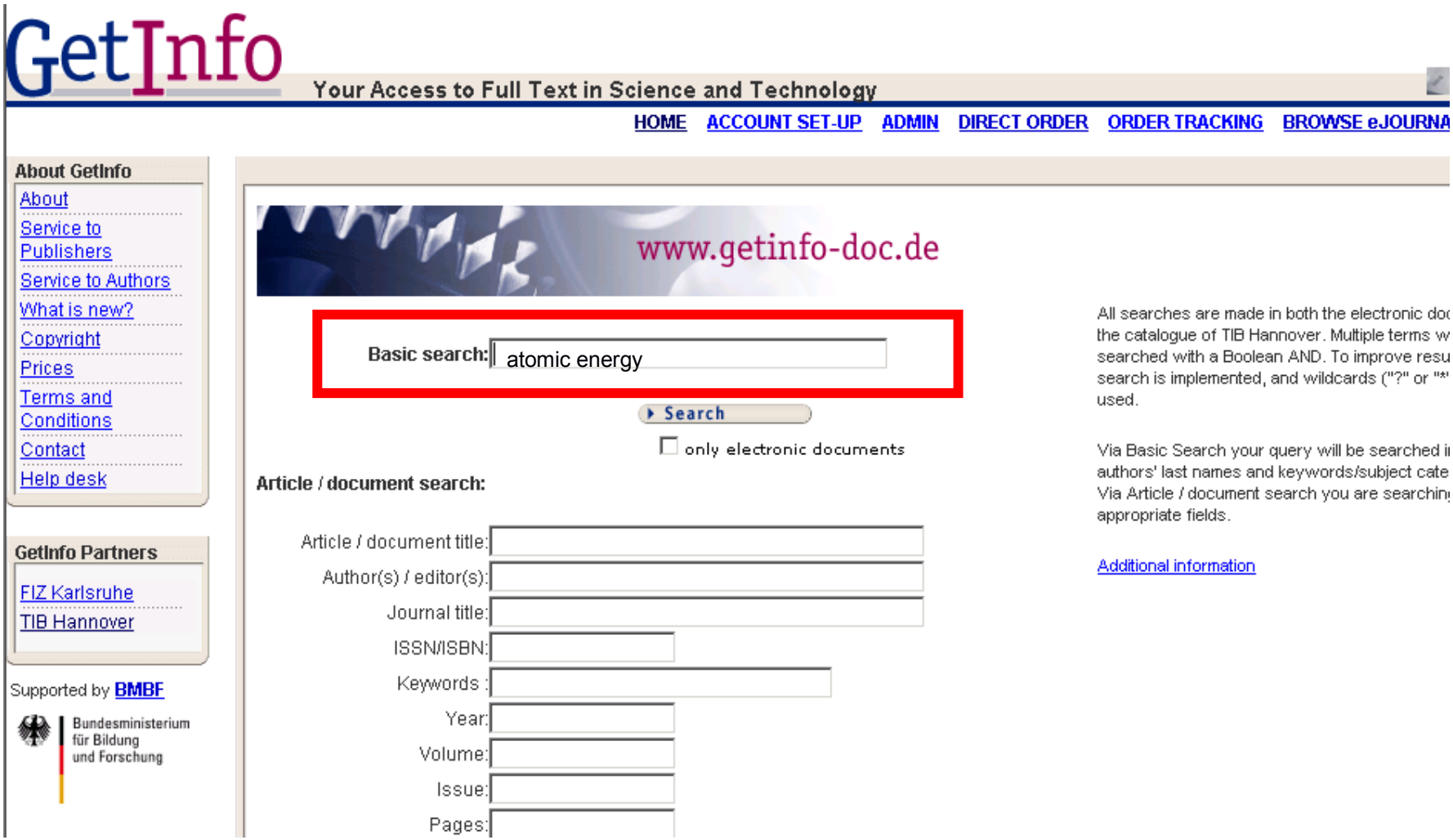
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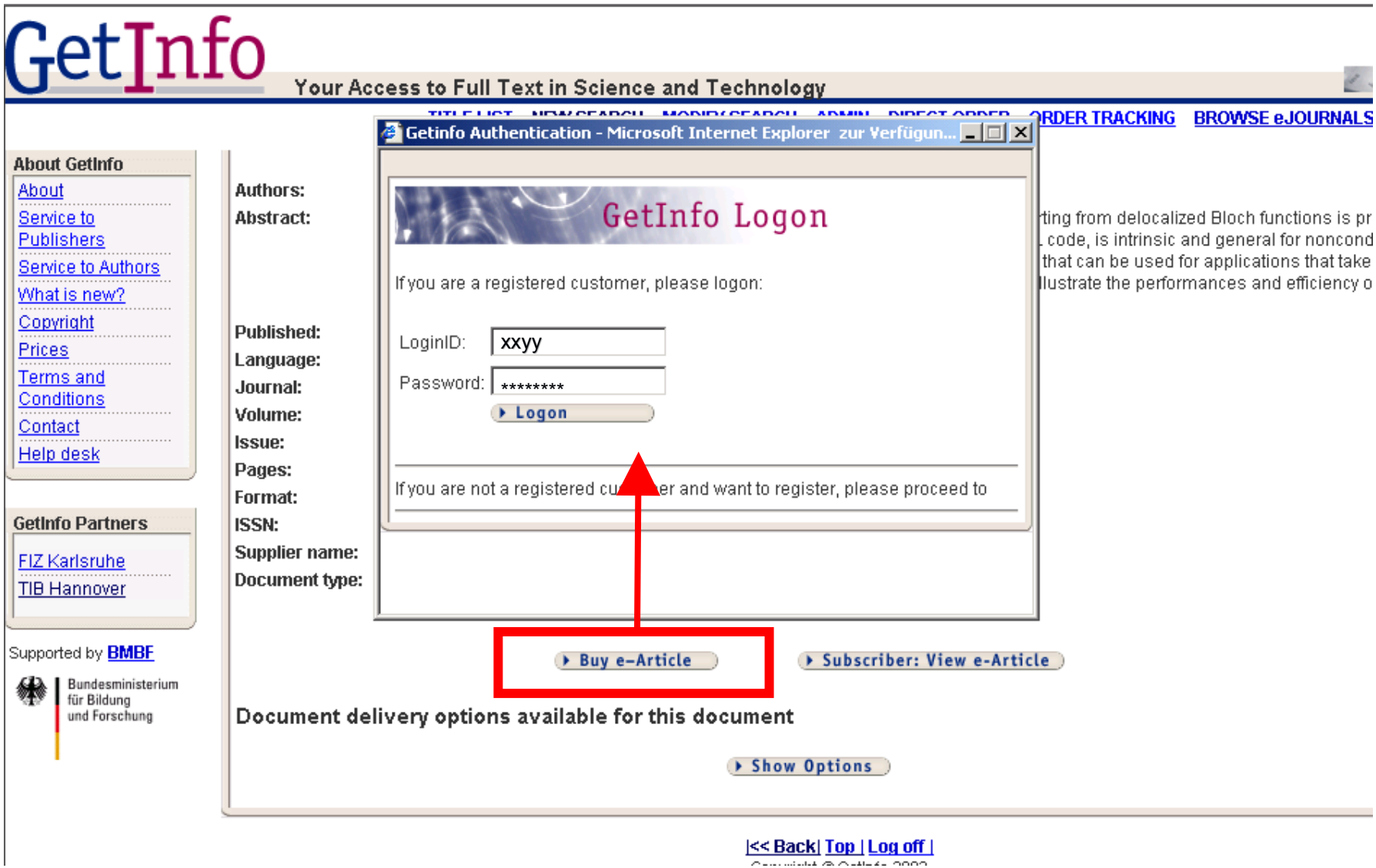
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A general method to obtain well localized Wannier functions for composite energy bands in linear combination of atomic orbital periodic calculations

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(Received 6 June 2001; accepted 17 September 2001)

A method for obtaining spatially localized crystalline orbitals starting from delocalized Bloch functions is proposed. The method, that has been implemented in the LCAO CRYSTAL code, is intrinsic and general for nonconducting systems, and provides a set of well localized Wannier functions that can be used for applications that take advantage of their localized character. Examples are given that illustrate the performances and efficiency of the proposed scheme. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1415745]

I. INTRODUCTION

In Hartree–Fock (HF) or Kohn–Sham theories it is a common practice to use canonical orbitals to construct the single-determinantal solution of a many-electron system. These orbitals are the eigenfunctions of a one-electron

in the molecular quantum chemistry literature to obtain orbitals maximally localized according to a given intrinsic and general criterion.[4–12] Perhaps the most widely used due to its relatively low computational cost (it scales as N^3) is the Foster–Boys method[4–6] that provides a set of orthonormal molecular orbitals for which the sum of their quadratic self

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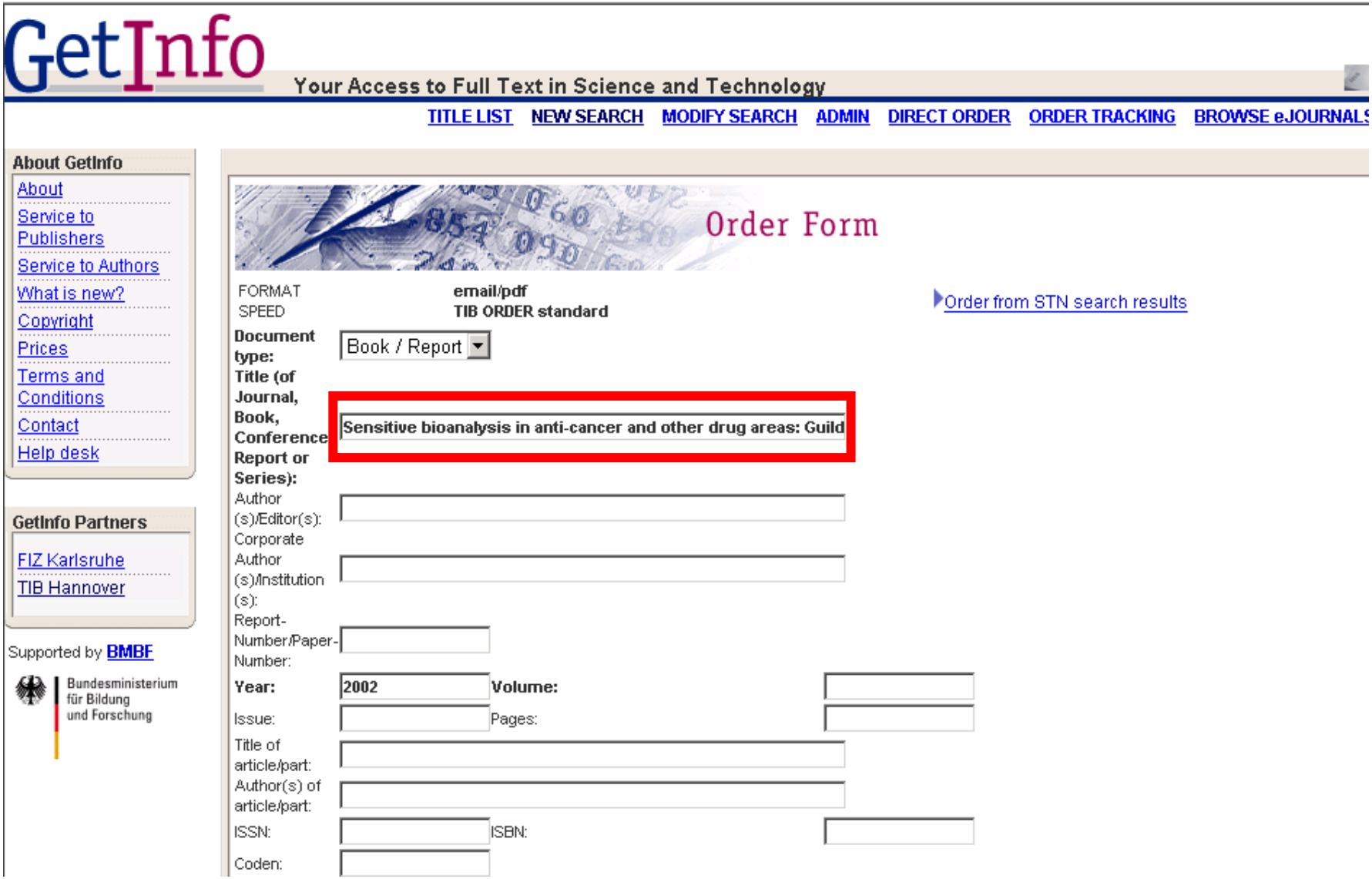
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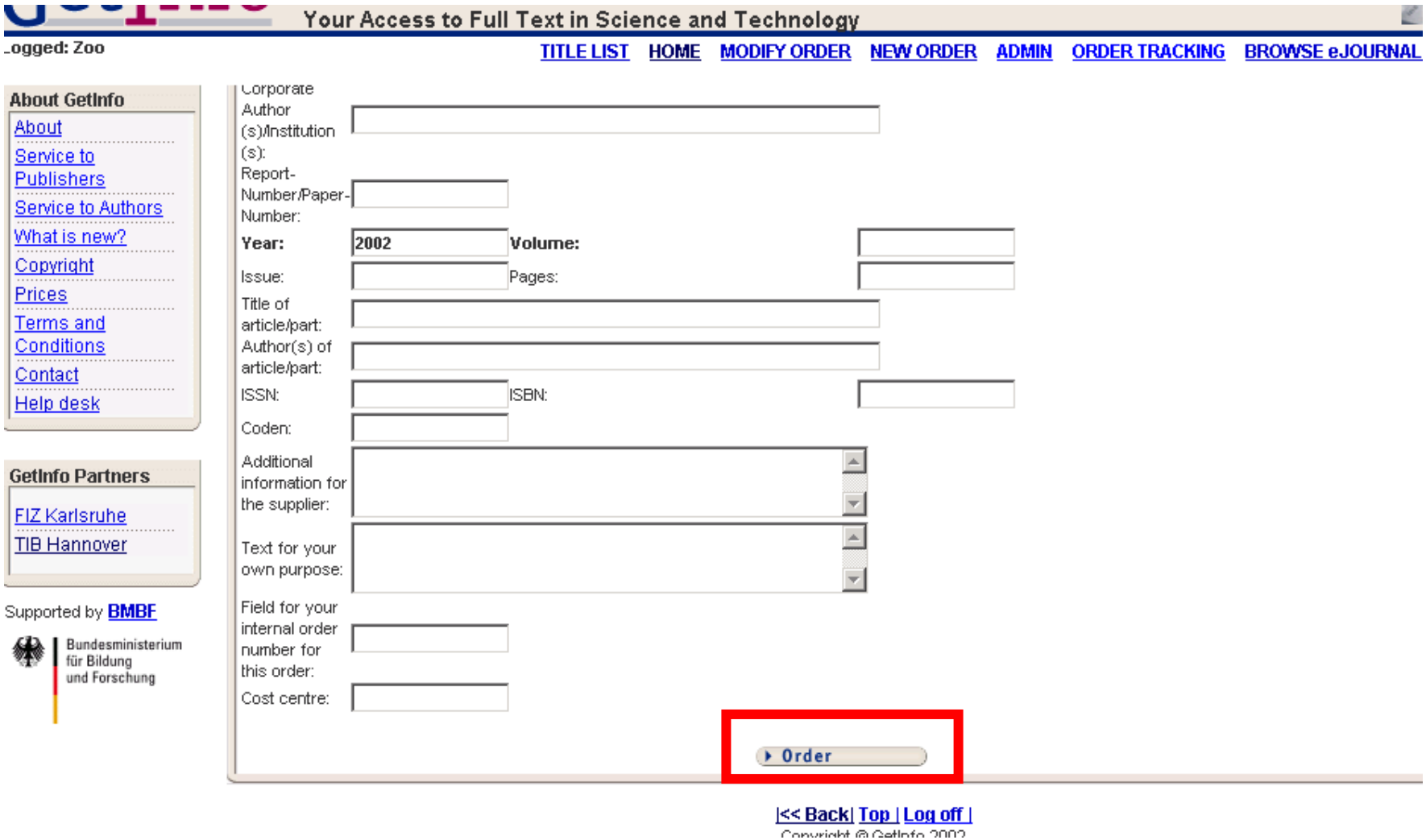
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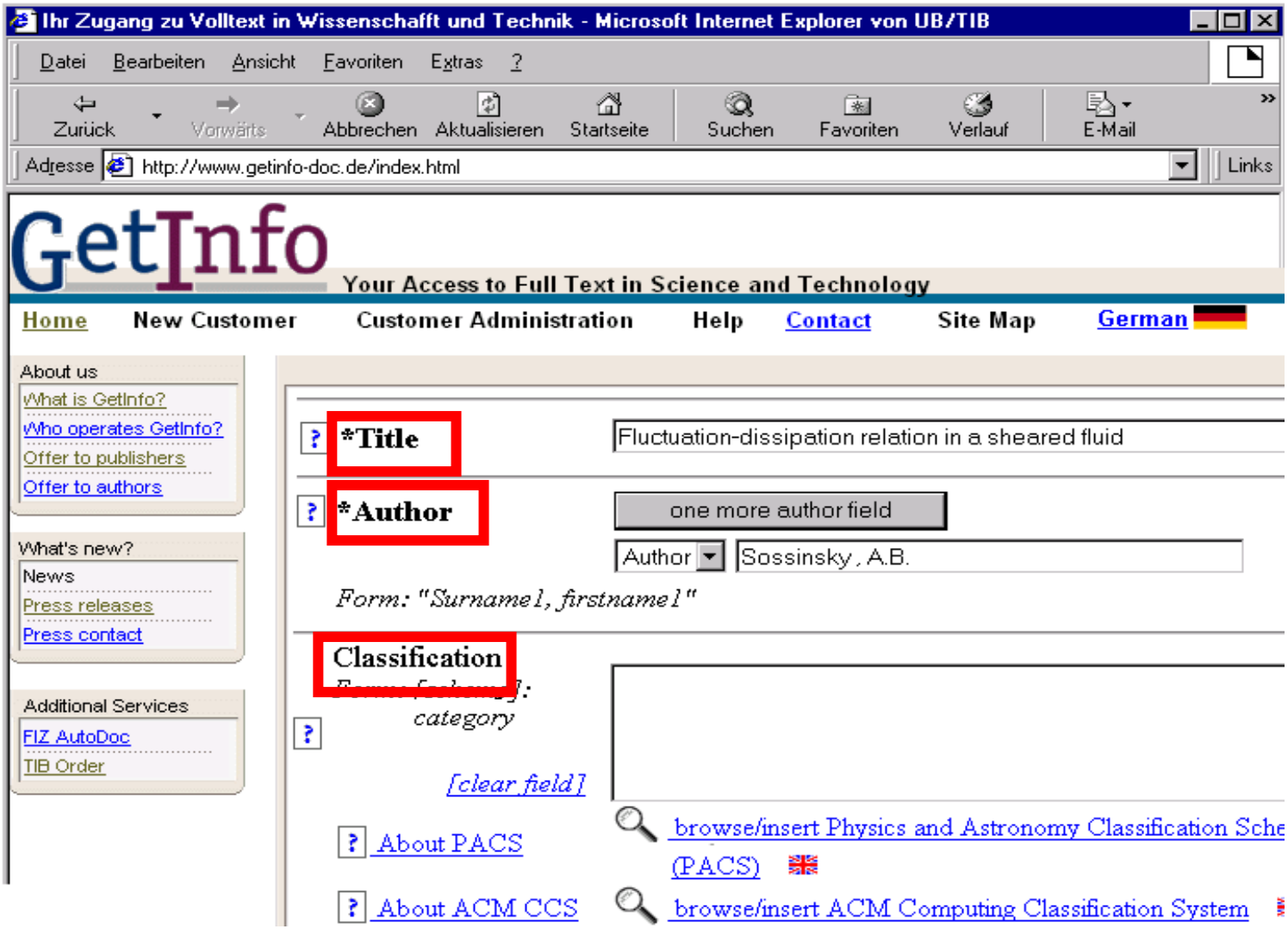
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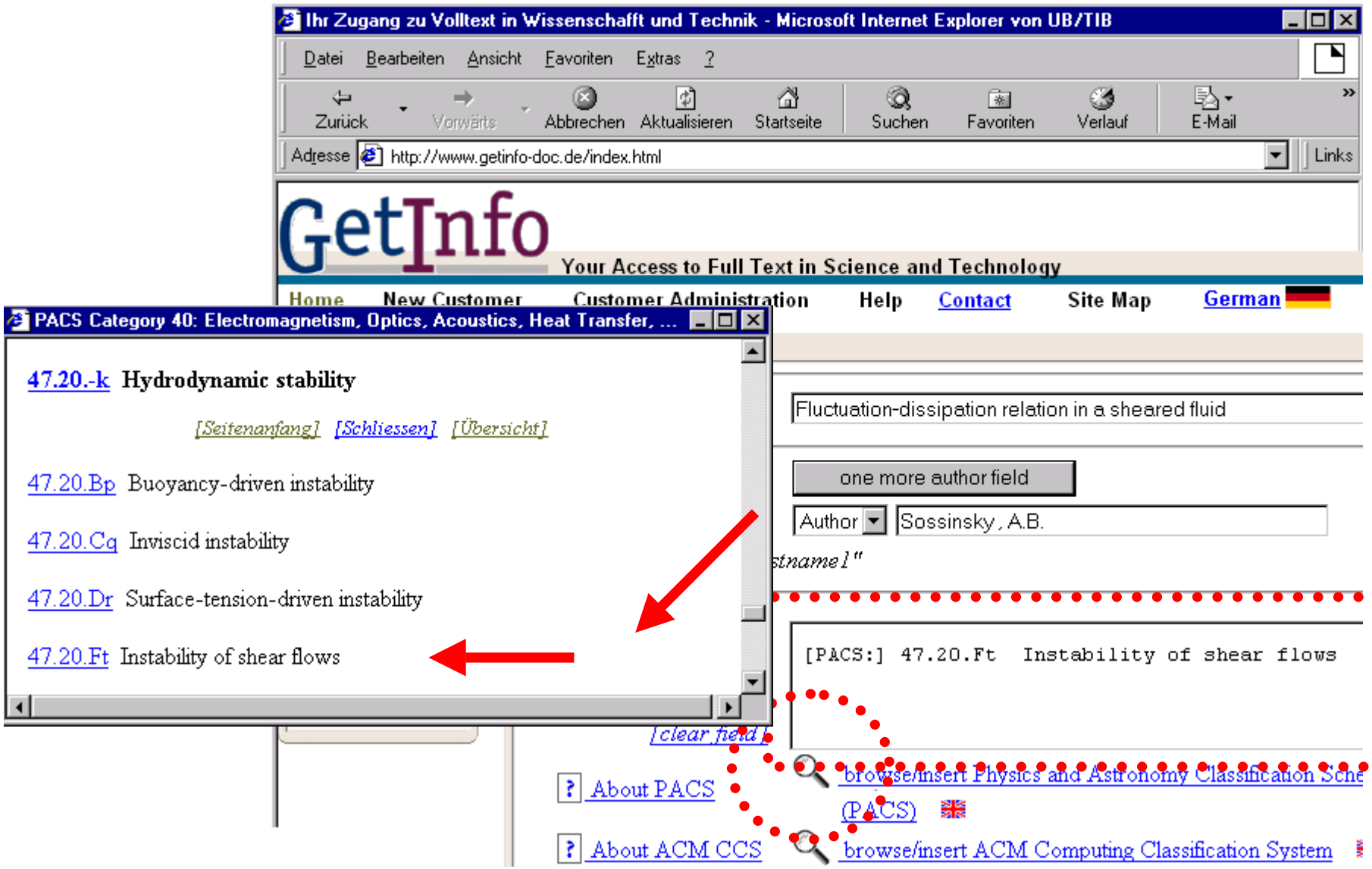
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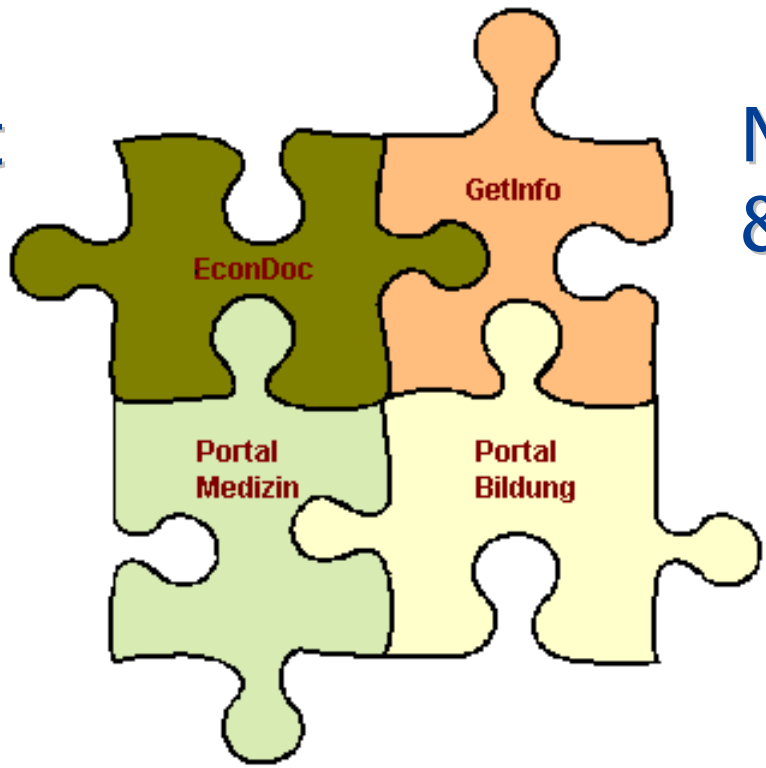

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