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*****************************  A U T O S U R F  ********************************
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   AUTOSURF Program Suite (v1.3)

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   This file is part of AUTOSURF.

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======                  Welcome to AUTOSURF Program Suite !                  ======
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 AUTOSURF is a freely distributed suite of codes for the automated construction of
 potential energy surfaces (PES) on vdW systems. The fitting algorithms implemented
 in the code are based on the L-IMLS methodology, and have many advanced features
 such as options for data-point placement, flexibility to include gradients in the
 fit, iterative refinement, and symmetry recognition. The code completely automate
 all the steps and procedures that go into fitting various classes of PESs and
 interfaces to popular electronic structure codes such as MOLPRO and GAUSSIAN.

 For non-commercial purposes, there is no charge to obtain AUTOSURF package for
 academic users (research institutes, universities, individuals), the user must
 simply sign a License Agreement. The License form can be obtained from the authors
 by email. The link for downloading the most recent version of AUTOSURF will be
 sent to the email address used in the License form.

 The package (v1.3) is composed of three main programs: AUTOSURF-ABI, AUTOSURF-PES,
 and AUTOSURF-PLOT:
 --> AUTOSURF-ABI performs guided surveys of the PES (various cuts), facilitating
 the benchmark of electronic structure methods, and the development of composite
 schemes such as complete basis set (CBS) extrapolation.
 --> AUTOSURF-PES carries out the automated construction of the PES to a user
 specified  accuracy target in a fairly black-box fashion: starting with a sparse
 set of initial ab initio seed points, the program grows a fitted PES over
 predefined ranges of energy and coordinates until the desired level of precision
 is reached.
 --> AUTOSURF-PLOT permits arbitrary evaluations of the PES, the generation of
 plots of 1D or 2D cuts of the surface (with optional relaxation) for any of the
 internal variables, and also to perform a variety of fitting error analyses in
 specified energy and coordinate ranges.

 In order to install and run AUTOSURF suite on a Linux system (Windows and OS X
 are currently not supported) you will need the following:
 * A Fortran90 compatible compiler.
 * MPICH or MPICH2.
 * The Fortran LAPACK Library.
 * Electronic structure code (MOLPRO and/or Gaussian).

 The standard AUTOSURF (v1.3) package is distributed as a compressed archive file
 named autosurf-v1.3.tar.gz, which includes the Fortran source codes of the three
 programs conforming AUTOSURF. Once the package have been downloaded, the user
 should simply unpack the file in the desired location and execute the corresponding
 Makefiles to generate the binaries (the Makefiles has to be modified according to
 the user's system requirements). The former is just a brief description of the
 installation procedure. Users should read AUTOSURF documentation for more detailed
 information.

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   Directory structure:
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   * BIN/           The compiled binaries.

   * DOC/           Documentation related to AUTOSURF.

   * EXAMPLES/      Documented examples + testing scenarios to check installation.

   * SOURCE/        The Fortran (77 & 90) source codes + Makefiles.
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   Please refer to the following files for further information:
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   * DOC/AUTHORS.txt:   The list of AUTOSURF developers.
   * DOC/CHANGES.txt:   Release Notes: history of modifications on each version.
   * DOC/COPYRIGHT.txt: The license under which AUTOSURF can be used.
   * DOC/INSTALL.txt:   Instructions to compile and install the program.
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   For more information, visit the web page:
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   https://makeapes.wixsite.com/autosurf
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